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THE UNIVERSITY OF ALBERTA
GENERALIZED COMPUTER DESIGN AND SIMULATION
OF SULPHUR PLANTS

by



RONALD SPENCER LEES

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled "Generalized Computer Design and Simulation of Sulphur Plants", submitted by Ronald Spencer Lees in partial fulfilment of the requirements for the degree of Master of Science.

Date.....April 30, 1970.....

ABSTRACT

A Fortran executive program has been developed for generalized process design and simulation calculations. This executive is completely general and is limited only by the equipment module subroutines available to it. The executive incorporates optimization of the ordering of the process calculations. This optimization involves analysis of the process flowsheet, and is done using an extension of a method presented in the literature.

The executive has been applied to the specific design and/or simulation of sulphur plants. The equipment module subroutines required for this application have been developed.

Stream compositions must be calculated throughout the sulphur plants and a thermodynamic equilibrium approach has been used. A generalized routine for determining equilibrium compositions involving large numbers of molecular species has been programmed. A method presented in the literature which is based on the concept of minimization of system free energy was utilized. In the application of this method, allowances have been made for the peculiarities of the sulphur recovery reaction system.

The developed program is user oriented. Data input is by free format and is as simplified as possible. Multi-level output is available to the user for controlling

the detail of calculation output.

A comparison of the program results for several sulphur plants has been done using the industrial data available. The results of this comparison are encouraging but not conclusive.

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I. INTRODUCTION

A shortage of sulphur, resulting from increased world demand, began to inflate sulphur prices beginning about 1964. Diminished sulphur stockpiles and improved sulphur production economics stimulated much interest in sulphur. Both existing and unused sources of sulphur were reviewed in the light of improved economic feasibility. Since that time production has remained high but sulphur demand and prices have peaked.

Interest in sulphur production as a by-product of sour natural gas processing has remained high in spite of the sulphur price slump. This is partly due to the continued high demand for natural gas. Presently some of the by-product sulphur accompanying sour natural gas must be stockpiled. The recent concern regarding air pollution has also sustained interest in sulphur. In sour gas processing care must be taken in plant design and operation to keep air pollution at tolerable levels. Attention has been focused on this problem both by governments and by the companies concerned.

In view of this active interest in sour gas sulphur production, the development of a generalized computer program for the design and simulation of such sulphur plants would seem to be a worthwhile project. This thesis describes such a program.

A. Sulphur Plant Description

Several methods of recovering sulphur from manufactured and natural gases have been developed. Goar(1) has concisely described these. Sulphur contained in sour natural gas is recovered exclusively by "dry bed catalytic conversion" processes and the scope of this thesis has accordingly been limited to processes of this type:

1. modified Claus
 - straight through process
 - split stream process
2. Direct Oxidation process
3. sulphur recycle process

Processing of sour natural gas includes removal of carbon dioxide and sulphur compounds, achieved using a gas treating process such as monoethanolamine. The extracted "acid gas" consists of hydrogen sulphide, carbon dioxide, water and small percentages of mercaptans, light hydrocarbons and aromatics. It is this acid gas which is the feed to the sulphur plant.

A detailed description of both gas treating and sulphur recovery, together with an extensive literature review can be found in Advances in Petroleum Chemistry and Refining(2).

1. Modified Claus Process

The modified Claus process is favoured for acid gas feeds containing more than fifteen mole percent hydrogen

sulphide. Burning one-third of the inlet hydrogen sulphide is the first step of the process. This results in a two to one ratio of hydrogen sulphide to sulphur dioxide throughout the rest of the plant. For feed streams with greater than twenty-five percent hydrogen sulphide, the "straight through" variation of the process is preferred. The whole feed is passed through a burner-waste heat boiler with sufficient air to burn all hydrocarbons and one third of the hydrogen sulphide. For more dilute feeds, difficulty in maintaining a stable flame is encountered. The alternate "split stream" process may then be used. In this case, one third of the feed is passed through the boiler with sufficient air to burn all hydrogen sulphide and hydrocarbons. The combusted stream is later combined with the unburned two thirds of the feed. This approach results in burning only one third of the total hydrocarbons, which is sometimes an important consideration. Reducing the hydrocarbons burned correspondingly reduces the undesirable formation of carbon, carbon disulphide and carbonyl sulphide.

Frequently if the boiler discharge contains a significant amount of converted sulphur, it is condensed out at this stage. This may increase overall recovery, particularly in the straight through process, but necessitates reheating the stream before catalytic conversion.

The second step of the Claus process involves two or

three stages of conversion. Each stage begins with reheating the partly combusted gas, using one of several options. A catalyst bed then converts some of the hydrogen sulphide and sulphur dioxide to elemental sulphur and water. The sulphur produced is recovered by condensation. Demister pads or a coalescer may be added to improve recovery of sulphur fog formed in the condensers.

Reheating the gas in preparation for catalytic conversion may be done in one of four ways:

- a. in-line burners
- b. hot-gas by-pass
- c. gas-to-gas exchangers
- d. indirect-fired heaters

The first two of these are preferred and have been included in this work. The last two are expensive and the trend is to use them less. They have not been included here.

The in-line burner option consists of burning a small fraction of the acid gas separately, and combining it with the stream to be heated. Hot-gas by-pass involves combining the stream to be heated with hot waste heat boiler gas - extracted before the primary exit.

Burning the residual gas in an incinerator is the last step of the process. The hot tail gas is vented to atmosphere via a stack.

The classical paper by Gamson and Elkins(3) describes the history of this process and the rationale of its

development. The important design and operation considerations are outlined.

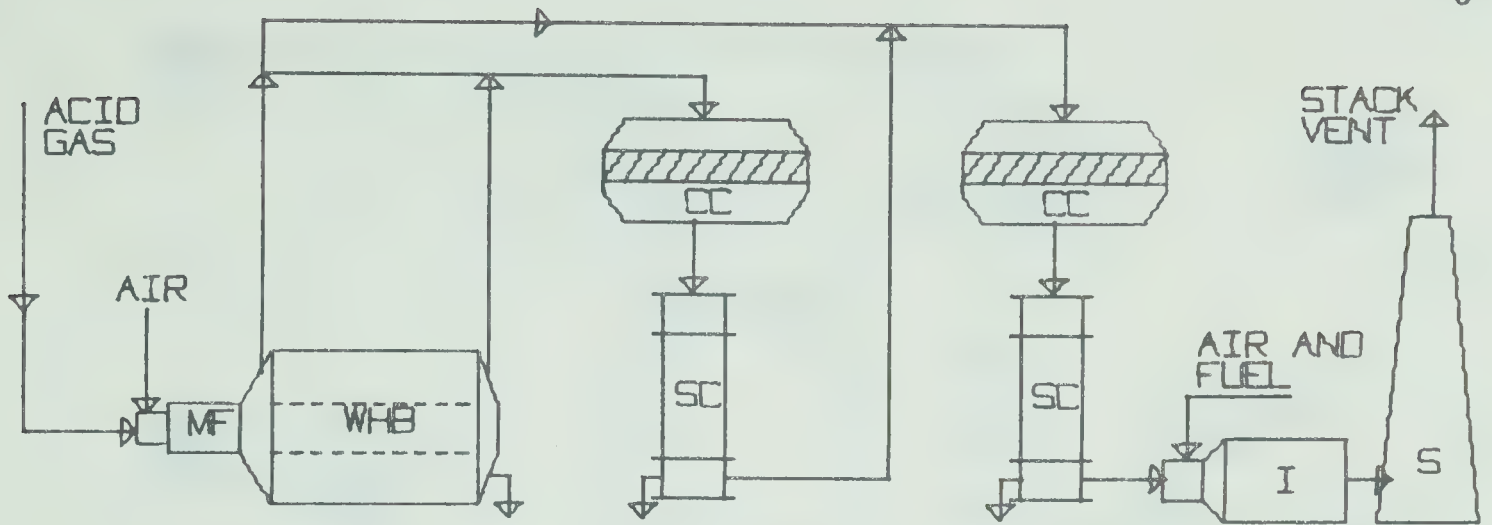
2. Direct Oxidation

Pan American Petroleum Corporation's Direct Oxidation process is sometimes used for low percentage hydrogen sulphide feeds. This process eliminates the waste heat boiler. Preheated acid gas is combined with air and fed directly into the first catalytic converter. From this stage on, the process resembles the Claus process except that air may be added before one or more converters to achieve conversion of hydrogen sulphide to sulphur.

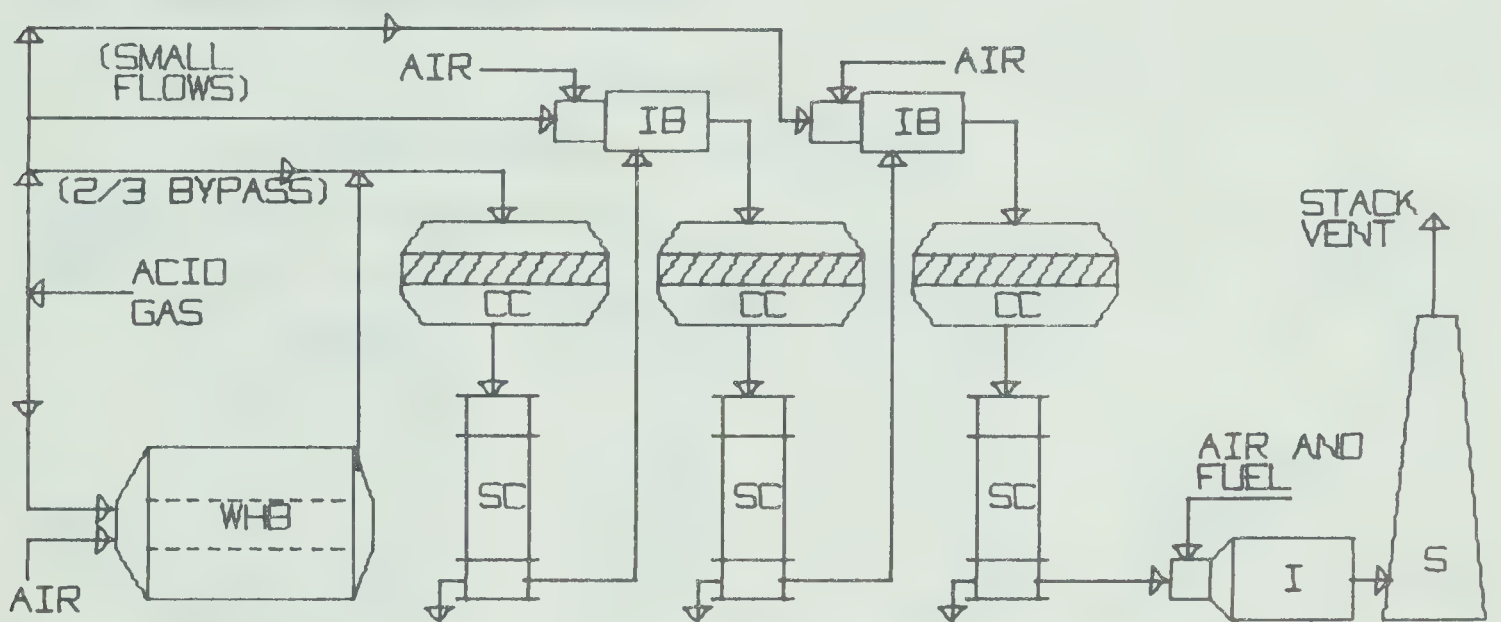
3. Sulphur Recycle

Jefferson Petrochemicals Canada Ltd. has developed a sulphur recycle process. This process is suitable for low hydrogen sulphide feeds, especially if significant amounts of hydrocarbons are present. None of the acid gas feed is burned in this process, avoiding the formation of troublesome carbon-sulphur compounds. Product sulphur recycled through a burner, is used to maintain a two to one ratio of hydrogen sulphide to sulphur dioxide. This burner stream, besides supplying a reactant, heats the feed to the first converter. The remainder of the plant is identical to the Claus type.

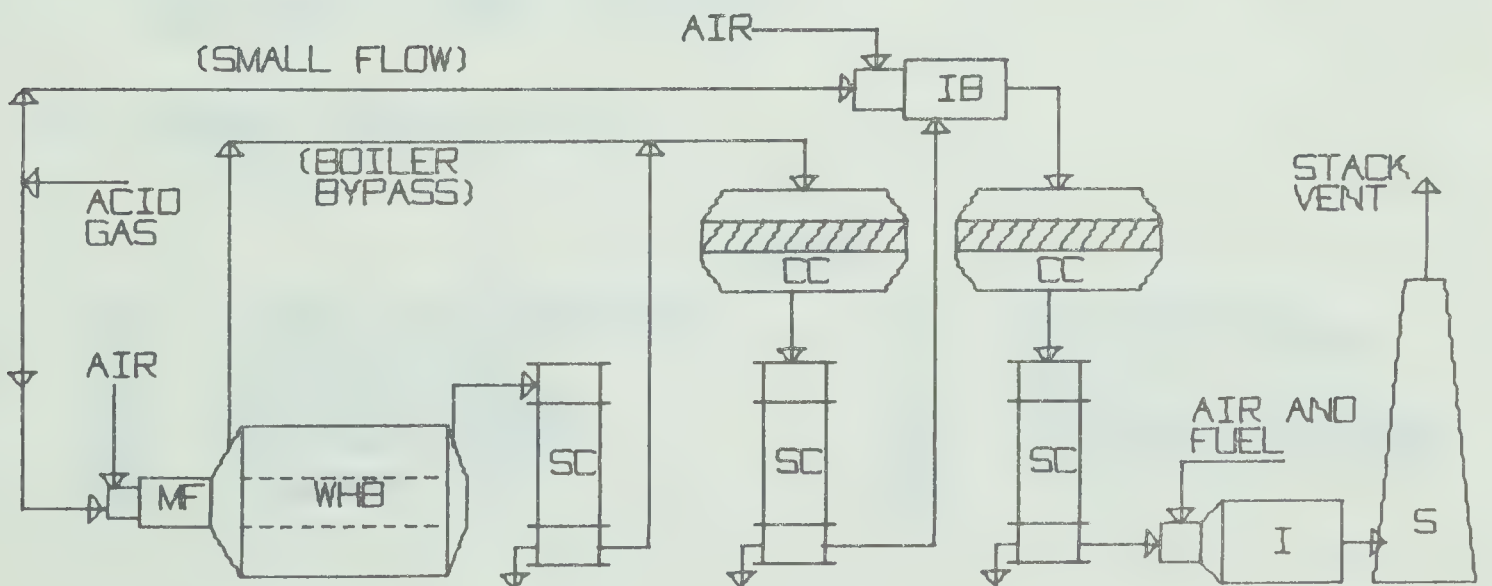
Several schematic sulphur plant flowsheets are illustrated in Figure 1.



A. STRAIGHT THROUGH CLAUS - REHEAT BY BOILER BYPASS.

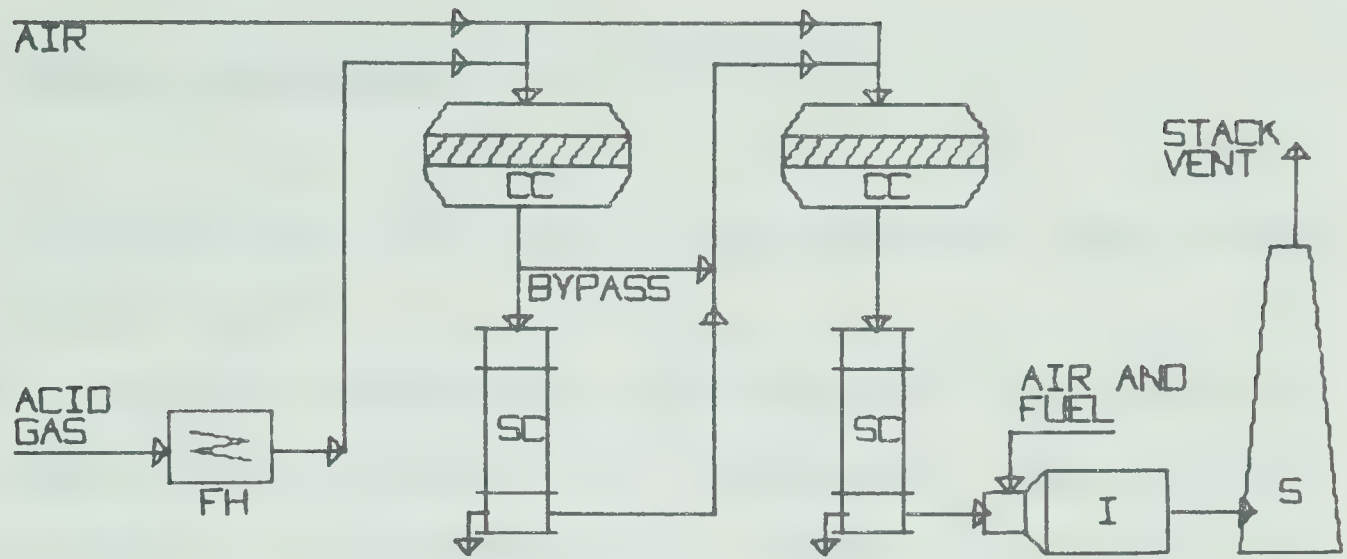


B. CLAUS 2/3 BYPASS - REHEAT BY IN-LINE BURNERS

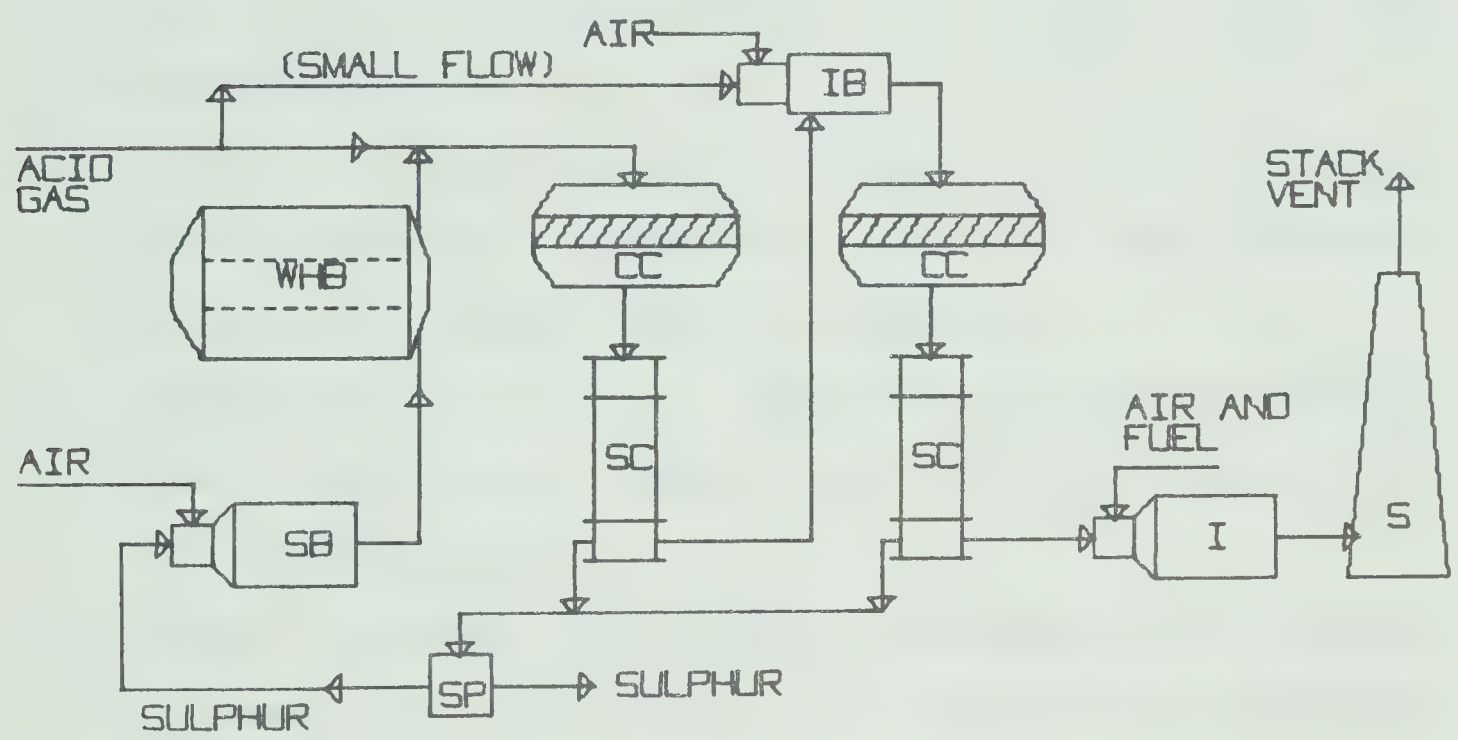


C. STRAIGHT THROUGH CLAUS - COMBINATION REHEATING.

..... (CONTINUED)



D. DIRECT OXIDATION PLANT.



E. SULPHUR RECYCLE PLANT.

LEGEND

- | | |
|--------------------------|-------------------------|
| CC - CATALYTIC CONVERTER | FH - FEED HEATER |
| I - INCINERATOR | IB - IN-LINE BURNER |
| MF - MUFFLE FURNACE | S - STACK |
| SB - SULPHUR BURNER | SC - SULPHUR CONDENSER |
| SP - SULPHUR PIT | WHB - WASTE HEAT BOILER |

FIG. I EXAMPLE SULPHUR PLANT FLOWSHEETS

B. Project Objectives

The objectives defined at the outset of this program development were:

1. To develop a generalized and versatile "executive" to serve as the framework for the program. This executive concept, to be explained in Chapter II, renders the program "flowsheet independent".
2. To incorporate optimization of the flowsheet calculation sequence.
3. To include those "equipment modules" necessary to design and/or simulate a variety of "dry bed catalytic conversion" sulphur recovery processes.
4. To utilize an efficient, dependable method for calculation of equilibrium compositions involving large numbers of molecular species.
5. To use rigorous calculations throughout the program, provided this was within the confines of reasonable computing times.
6. To emphasize user orientation of the program. Towards this end, data input was to be as simplified as possible, data error checks and error messages were to be used extensively and multi-level output was to be incorporated for the user's benefit.
7. To compare the program results with industrial data to confirm the program's usefulness.

The initial program development began using an I.B.M. 1800 time sharing system. This system is limited to Fortran II and the initial programming was so limited. Later, when the program became too large for this system, from both program storage requirements and execution time standpoints, development was transferred to the Computing Services I.B.M. 360/67 system. Even though up to date Fortran was available here, Fortran II was maintained to preserve continuity. All program listings, execution output and the thesis body proper were produced using the CP/CMS time sharing monitor system.

II. EXECUTIVE PROGRAM DEVELOPMENT

A. Executive Programming Concept

The variety of sulphur plant flowsheets that must be accommodated by the proposed program necessitates an executive of some form. Using the process flowsheet, the executive directs if and when program functions are done.

It was decided that the executive developed should in no way be inherently restricted to sulphur plant design and simulation. Rather, it should only be limited by the equipment modules available to it. A module in this context refers to an independent group of subroutines which performs a particular task. An equipment module is used to either design or simulate one type of equipment (one or more physical pieces of equipment). Thus, to apply the executive to sulphur plants, the only requirement is that the necessary modules be included.

The concept of an executive program to manage process calculations is not new and many have been developed. Some of these are briefly discussed in the literature review in the following section. There has been a continuous evolution from hand computation to sophisticated executives.

With the advent of computers used for engineering calculations, repeated hand computation was replaced with special purpose programs. The most efficient means of doing a single type of problem could be utilized in these

programs. However, they were very inflexible and a minor problem change necessitated a new program, or at least a modification of an existing one. It was a desire for flexibility that provoked the concept of executive programming. The only difference between various process calculations using this technique would be the encoded flowsheet data and perhaps the equipment modules. The generality produced using the executive approach substantially increases flexibility, but inherently compromises efficiency in most specific problems.

The primary function of the executive program is to replace the engineer as the decision-maker, at least as far as the calculations are concerned. The executive directly controls the order of equipment calculations and supervises data input, output of results and calculation bookkeeping. If iteration on process recycle loops is required, as it usually is, the executive must repeat the calculations at the appropriate time and detect when convergence is achieved.

The most primitive executives rely on a calculation sequence supplied as data. More advanced programs devise their own feasible ordering of calculations, either as the calculations proceed or beforehand. The additional sophistication of calculation sequence optimization may be incorporated into the executive to improve efficiency and convergence. In this event, the optimum sequence should be established before the equipment calculations are begun. The

calculation starting point is an integral part of the optimum, and starting at an arbitrary point in the flowsheet may preclude using the optimum sequence.

Once the executive has been developed, the modules it requires to complete the desired calculations must be supplied. Although these modules must be compatible with the executive, they are essentially independent program packages. Some of them are actually sub-executives which temporarily maintain program control. The following modules have been developed and included with the present executive program:

1. data input module (Chapter V.)
2. calculation sequence optimization module (Chapter II.)
3. equilibrium composition module (Chapter III.)
4. process calculation summary module (Chapter V.)
- 5-13 equipment modules (Chapter IV.)

Because of their distinctive nature, each module will be described individually.

B. Literature Survey

Since the innovation of the executive programs, there has been a steady increase in their sophistication, capability and objectives. The first ones to appear, such as Kellogg's "Flexible Flowsheet"(4) and I.B.M.'s GIFS(5), required specification of the computational sequence as part of the input data. Even though more flexible than the

special purpose programs, they merely called the provided routines in the specified order and maintained iteration bookkeeping.

The first version of PACER(6) was more ambitious. A feasible computational ordering could be supplied, but in lieu of this, the executive would attempt to find a feasible path, making recycle assumptions as necessary. The calculation path-seeking took place after each "equipment block" calculation. On recycling, the same search took place again. This version of PACER made no attempt to optimize the order of the calculations.

Many attempts have been made to find effective ways of optimizing calculation sequences. This task is complicated by process recycle loops and by stability and convergence considerations. A systematic analysis of the calculation network is necessary to achieve optimality. Extensive work on analysis of recycle-process calculation networks has been done. Basically there are two different approaches, with a third being a combination of the two.

The first of these is the direct method, whereby the equations describing the process are formulated and the resulting set is solved simultaneously. Solution is normally achieved with an iterative technique utilizing linearized equations. Rosen(7) whose work was based on the previous work of Nagiev(8,9), devised a method using this approach. The direct method fails to take advantage of problem structure which could be used to simplify the problem. For

large problems, simultaneous solution of many equations becomes an impractical task. Since this approach attacks the whole problem at once, the only possible use for an executive function is in formulating and grouping the system equations.

The second approach, which does take account of problem structure, is known as the "tearing" method or successive substitution. Methods using this approach assume quantities necessary to make the initial calculations, follow the process flow and subsequently find improved values of the assumed quantities. Iteration is necessary to arrive at a converged solution. This procedure is identical to that used by an engineer doing the calculations by hand, and lends itself to the use of an executive.

The rate at which the overall process calculation converges is related to the number of recycle parameters assumed and iterated upon. As a result, much study has been devoted to ordering calculations to minimize recycle assumptions. This minimization is the most common criterion for calculation sequence optimizing.

Most methods of the second type involve matrix representation of the process flowsheet. Lee and Rudd(10) have devised a four algorithm method that assumes previous identification of the recycle loops. The method seems to be conceptionally sound but difficult to implement. Norman(11) has presented a matrix method using Boolean algebra which can be used to identify the recycle loops of a process. A

method by Rubin(12) uses a special process matrix to obtain at least a local minimum for the desired optimization. Sargent and Westberg(13) dislike the inefficient use of computer space involved in the matrix methods. They have devised a two step method of ordering. Using an algorithm, the process is first broken into groups of units. Then the units within each group are optimally ordered using dynamic programming.

Ravicz and Norman(14) and Naphtali(15) have developed similar combinations of the two approaches. Using these methods, the parts of the process excluding recycle loops are solved sequentially. The remaining recycle portions are solved simultaneously.

Himmelblau and Bischoff(16) describe a method similar to Norman's(11) for identifying recycle loops and apply Boolean algebra to algebraic equations as well as to equipment units. A method of "precedence ordering" is described and signal flow graph theory is applied to recycle networks.

Rudd and Watson(17), besides outlining a design philosophy in their text, give an algorithm for design variable selection. The method presupposes the designer is at liberty to interchange design and stream specifications, which is not usually true. Methods of attacking macro-systems are outlined. These methods may have application to single processes as well.

Most recycle network analyses (and therefore derived executives) assume a common "rule of calculations": outputs

should be calculated from inputs for all equipment. Computational stability has been shown to be much greater for forward calculations than for backward ones.(17,18) If this rule is strongly adhered to, it is quite restrictive. For instance, process feed unknowns and product specifications are eliminated. This restriction can largely be overcome by integrating a "material and/or energy balance envelope" program with the executive as done by Nieman(19) using the PACER executive. This program feature has not been included in the executive developed for this project.

Process optimization is another refinement that may be added to the executive. Although little seems to have been published on Shell's CHEOPS, it apparently has this feature to some extent. Intentions to include this phase in SPEED-UP(13) and later versions of PACER(20) have been stated. The approaches to process optimization are dynamic programming(17) for the acyclic cases and either non-linear programming(21) or hill climbing techniques(17) for processes involving recycle. Process optimization is beyond the scope of the present work.

A more extensive list of executive programs may be found in the text by Rudd and Watson(17). Cavette(22) has presented a comprehensive review of numerical methods used for solving recycle processes.

C. Optimization of Calculation Sequence

None of the methods for optimizing recycle networks presented in the Literature were considered suitable for the present executive's needs. The possibility of using one of these methods as a starting point for the development of a new method was explored. It was found that Rubin's Method(12) showed the most promise in this regard.

1. Rubin's Optimizing Strategy

Rubin's method will not be described in detail since it is the underlying principles that are of primary interest. For a detailed description of his method, and examples of its use, the reader is referred to the original paper.

Rubin utilizes a modified form of the process "association" matrix. The process equipment units are denoted as nodes $N(k)$, ($k=1,2,...,n$) which are connected by the flowsheet streams $S(j)$, ($j=1,2,...,n$). Associated with each stream are $U(j)$, ($j=1,2,...,n$) stream unknowns. A particular sequence of these nodes represents an order of process calculations. The nodal sequence is denoted as $N(k)<i>$, ($i=1,2,...,n$), where the k th process node $N(k)$ is the i th node in the sequence. The corresponding association matrix is formed as follows:

A is an $n \times n$ association matrix, with

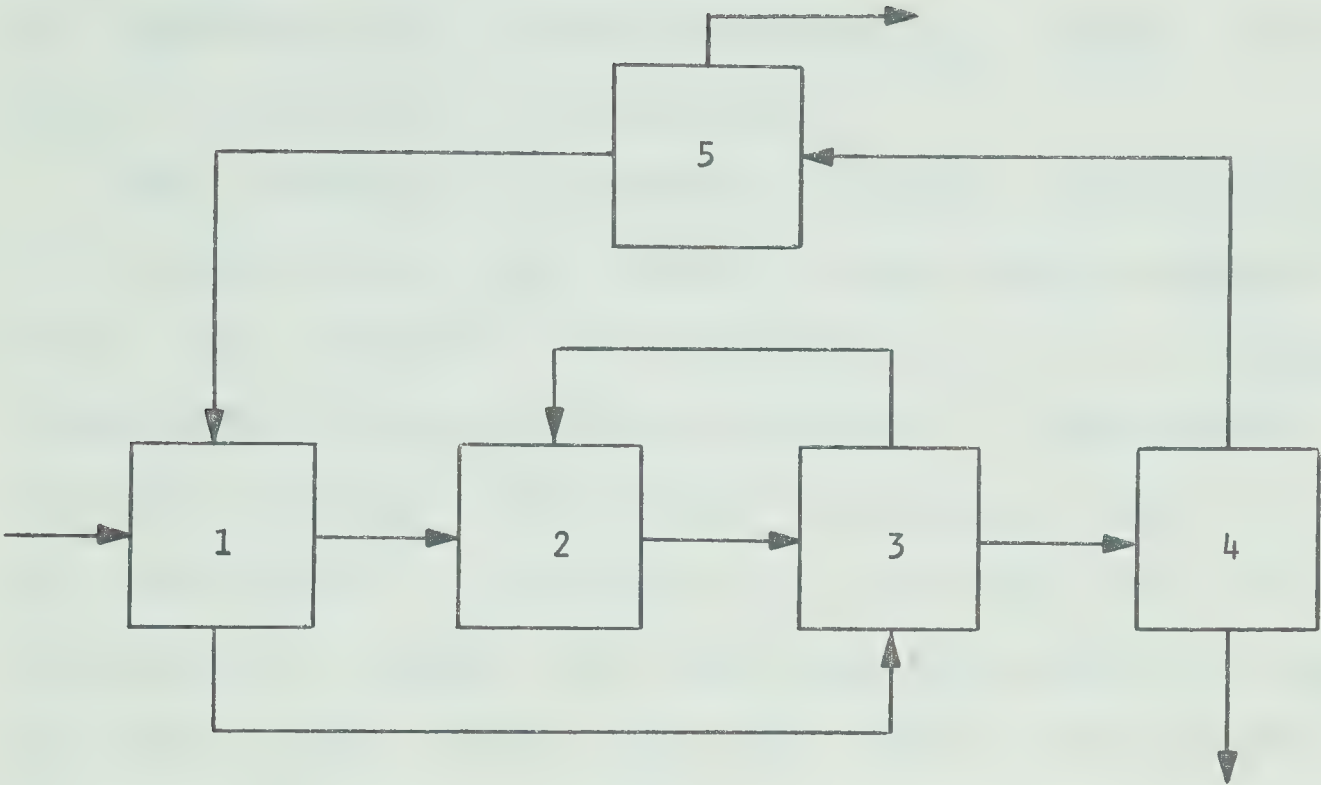
$A(i,j) = 0$ if no stream exists from $N(k)\langle j \rangle$ to $N(k)\langle i \rangle$

$A(i,j) = U(1)$ if stream 1 exists from $N(k)\langle j \rangle$ to $N(k)\langle i \rangle$

A simple process and the association matrices resulting from two nodal sequences for this process are illustrated in Figure 11. It will be noted that feed and product streams are not represented in the matrix and are ignored in the analysis. Also it should be noted that "self loops" (diagonal entries) are not allowed.

In the association matrix, the number of stream parameters that must be assumed for the related nodal sequence appear above the diagonal. Rubin uses the minimum recycle assumptions criterion for optimizing the sequence. This criterion is met if the sum of the elements above the diagonal is a minimum. A different criterion of optimality can easily be used by attaching a different significance to the $U(j)$'s. For instance, $U(j)$ could become the weighted difficulty or weighted sensitivity of calculating stream $S(j)$.

Rubin attempts to minimize the upper triangular sum of the association matrix by a systematic exchanging of nodal positions in the sequence. He gives a description of a complicated procedure for finding the most profitable exchange. This procedure will not be described here. The mechanics of both sequence position exchanging as well as other sequence changes will be explained with the modified method. The effect of exchanging two positions in a nodal sequence is illustrated in Figure 11. It can be seen that



A. - Process flowsheet (one unknown parameter associated with each stream in this case).

N(k)	(2)	(4)	(5)	(3)	(1)
(2)	.	0	0	1	1
(4)	0	.	0	1	0
(5)	0	1	.	0	0
(3)	1	0	0	.	1
(1)	0	0	1	0	.

N(k)	(3)	(4)	(5)	(2)	(1)
(3)	.	0	0	1	1
(4)	1	.	0	0	0
(5)	0	1	.	0	0
(2)	1	0	0	.	1
(1)	0	0	1	0	.

B. - Association matrices for two calculation sequences.

FIG. 11 A SIMPLE PROCESS FLOWSHEET AND TWO CORRESPONDING ASSOCIATION MATRICES

in the example shown, exchanging nodes $N(2)\langle 1 \rangle$ and $N(3)\langle 4 \rangle$ in sequence 1 to produce sequence 2, results in a net reduction of recycle assumptions.

The sequential exchanging of nodal positions is the only modification Rubin makes to the nodal sequence. He gives two criteria for termination of this exchanging. These are not used in the new method. Rubin admits the method is empirical and without rigorous mathematical proof. He even gives an example of a flowsheet for which the optimum is not found. The method was programmed as presented by Rubin and several difficult process flowsheets were formulated. Several problems were encountered in using the original method and are described below.

1. While Rubin's method usually improved an arbitrary initial sequence, it failed to reach the true optimum for any of the examples tried.
2. The sequence changes frequently became periodic after a certain point. Alternating between two sequences is prevented by an algorithm stipulation. However, a repeated series of three or more sequences is not prevented and when this cycling occurs the completion criteria were never met.
3. Rubin suggests that when the algorithm is completed, the final sequence may be reversed and the algorithm re-applied. The resulting best sequence may be more optimal than one obtained with a single application of the algorithm. When repeated reversal of final sequence

was tried in an effort to reach the true optimum, these sequences were found to repeat.

4. The method inherently has great difficulty in moving groups of nodes within the sequence. Thus, even if moving such a group would be advantageous the method often fails to do this, since it is limited to exchanging two nodes at a time. A string of nodes connected by single streams is an example of this. Moving any one of the nodes within the string may adversely effect the sequence, but moving the whole string may significantly improve it. It was suspected that this problem often accounted for the method failing to reach the optimal sequence.

Because of these problems, Rubin's method was considered inadequate. Many modifications to his method were tried in an attempt to find a procedure which would quickly and dependably find an optimum calculation sequence. Several of these modifications were very successful.

2. The New Optimization Technique

The new optimization method developed can be logically broken into three parts:

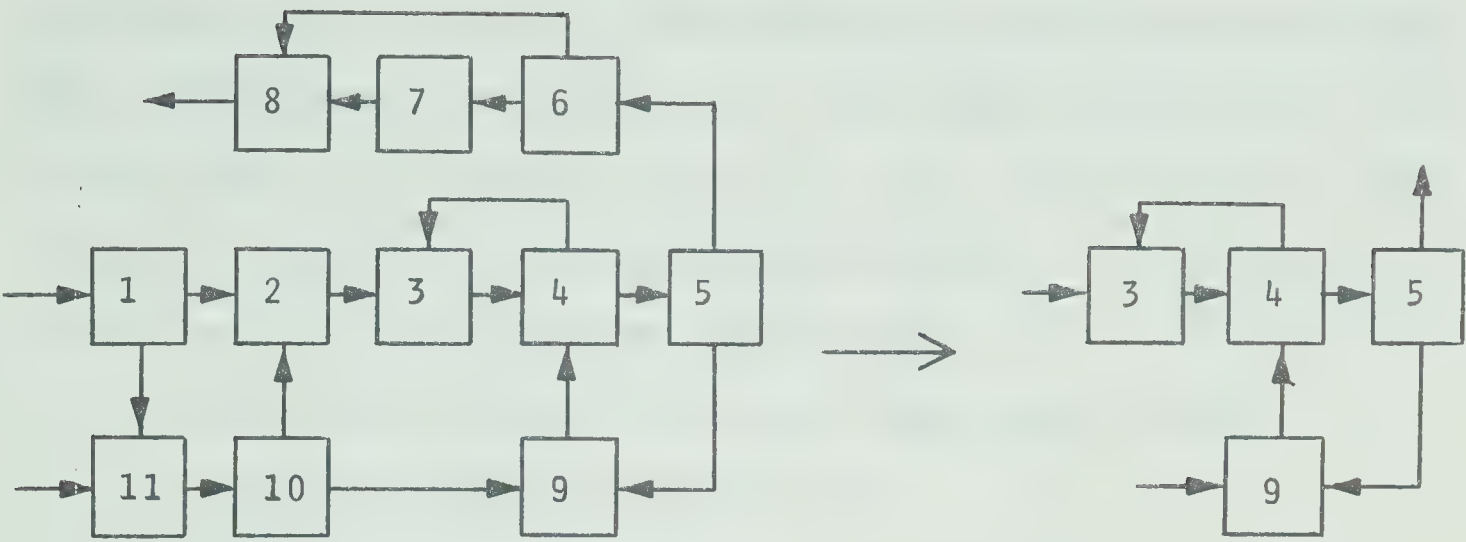
- a. flowsheet simplification
- b. nodal sequence modification
- c. randomization and termination.

a. Flowsheet Simplification

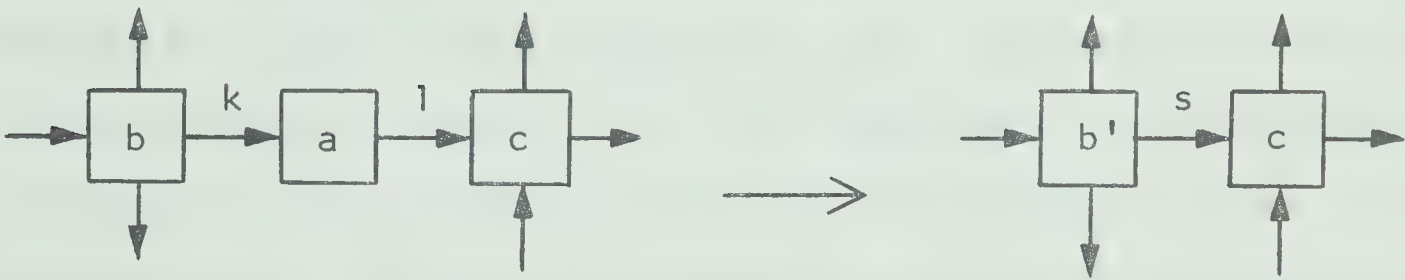
Often the search for the optimum sequence is made difficult by flowsheet complications which can be simplified. Such a simplification consists of "reducing" the flowsheet by eliminating nodes which are irrelevant from an optimization standpoint. However, care must be taken not to obscure or eliminate the true optimum by such a flowsheet reduction (ie. the optimum of the simplified flowsheet must correspond to the original flowsheet optimum). Several flowsheet reduction criteria were tried. The following two step procedure was found satisfactory.

Phase 1 consists of eliminating from optimization consideration those nodes which are extraneous to the recycle portion of the flowsheet. This is done using a procedure similar to the "precedence ordering" described by Himmelblau(16). Nodes without antecedents and then those without descendants are successively eliminated. Hence in Figure III-A nodes 1 - 11 - 10 - 2, can be eliminated in turn since they lack antecedents. They are placed in that order at the beginning of the final calculation sequence. Similarly nodes 6 - 7 - 8 can be eliminated, since they lack descendants, and placed at the end of the sequence. Optimization then, is concerned only with the ordering of nodes 3 - 4 - 5 - 9.

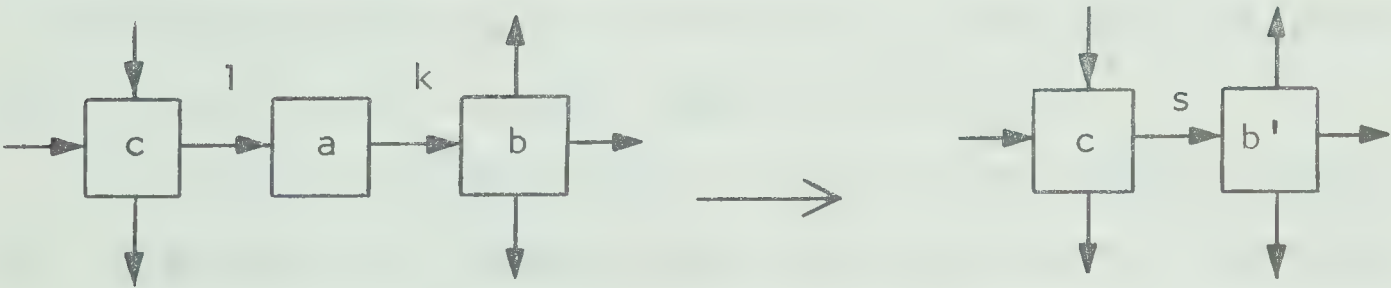
Phase 2 of the flowsheet simplification is concerned with grouping of nodes to form single nodes. A node may be



A. - Elimination of nodes extraneous to recycle network.



B. - Forward reduction - elimination of node N(a).



C. - Backward reduction - elimination of node N(a).

FIG. III FLOWSHEET SIMPLIFICATIONS

eliminated if it can be replaced by a single pseudo-stream. The conditions required for the node elimination are illustrated in Figure III-(B & C). Referring to this figure, forward or backward elimination of node $N(a)$ by combining it with node $N(b)$ may be done if:

- $N(a)$ has only one input and one output, and
- $N(b)$ has only one input, and
- $U(l)$ is less than or equal to $U(k)$.

All possible forward eliminations are done first. A string of two or more nodes similar to $N(a)$ may be combined to form a single node by repeated use of this elimination. When this has been completed, any possible backward eliminations are done. It will be noted that backward elimination will result in groups of two nodes at most, and that $N(a)$ in Figure III-C. cannot be eliminated by forward elimination.

After each elimination of a node, a link relating the true flowsheet to the simplified one is saved. Stream $S(k)$ is eliminated and pseudo-stream $S(s)$, identical to stream $S(l)$ is introduced between nodes $N(b)$ and $N(c)$.

It should be emphasized here that the simplification of the flowsheet is temporary and for optimization purposes only. Once optimization has been completed, the actual flowsheet is restored. The final calculation sequence is derived from the optimum reduced flowsheet using the links stored during node elimination.

The flowsheet reduction technique was found to greatly

aid the optimization. The fourth problem mentioned regarding Rubin's method was entirely eliminated.

b. Nodal Sequence Modification

Three sequence modifications were implemented in the new method:

- nodal exchange,
- nodal promotion, and
- nodal demotion.

The mechanical effect of these modifications on the association matrix are illustrated in Figure IV. It can be seen that some matrix elements "cross" the diagonal. It is desirable if this results in a decrease in the upper triangular sum of the matrix. The decrease in this sum that will result from the sequence modifications can be evaluated as follows:

if $E(i,j)$ is the decrease in the upper triangular sum resulting from exchanging the nodes in positions i and j ,
 $P(i,j)$ from promoting the node in position i to j ,
 $D(i,j)$ from demoting position j to i ,

$$\text{then } E(i,j) = \sum_{k=i+1}^{k=j} (A(i,k) - A(k,i)) + \sum_{k=i+1}^{k=j-1} (A(k,j) - A(j,k)),$$

$$P(i,j) = \sum_{k=i}^{k=j-1} (A(k,j) - A(j,k)), \text{ and}$$

N(k)	(1)	(2)	(3)	(4)	(5)		N(k)	(1)	(4)	(3)	(2)	(5)
(1)	11	12	13	14	15		(1)	11	14	13	12	15
(2)	21	22	23	24	25		(4)	41	44	<u>43</u>	<u>42</u>	45
(3)	31	32	33	34	35	→	(3)	31	<u>34</u>	33	<u>32</u>	35
(4)	41	42	43	44	45		(2)	21	<u>24</u>	<u>23</u>	22	25
(5)	51	52	53	54	55		(5)	51	54	53	52	55

A. - Sequence "exchange" of positions 2 and 4.

N(k)	(1)	(2)	(3)	(4)	(5)		N(k)	(1)	(4)	(2)	(3)	(5)
(1)	11	12	13	14	15		(1)	11	14	12	13	15
(2)	21	22	23	24	25		(4)	41	44	<u>42</u>	<u>43</u>	45
(3)	31	32	33	34	35	→	(2)	21	<u>24</u>	22	23	25
(4)	41	42	43	44	45		(3)	31	<u>34</u>	32	33	35
(5)	51	52	53	54	55		(5)	51	54	52	53	55

B. - Sequence "promotion" of position 4 to position 2.

N(k)	(1)	(2)	(3)	(4)	(5)		N(k)	(1)	(3)	(4)	(2)	(5)
(1)	11	12	13	14	15		(1)	11	13	14	12	15
(2)	21	22	23	24	25		(3)	31	33	34	<u>32</u>	35
(3)	31	32	33	34	35	→	(4)	41	43	44	<u>42</u>	45
(4)	41	42	43	44	45		(2)	21	<u>23</u>	<u>24</u>	22	25
(5)	51	52	53	54	55		(5)	51	53	54	52	55

C. - Sequence "demotion" of position 2 to position 4.

(Note: elements crossing the diagonal are underlined.)

FIG. IV CALCULATION SEQUENCE MODIFICATIONS

$$D(i,j) = \sum_{k=i+1}^{k=j} (A(i,k) - A(k,i)) \quad .$$

also, $E(i,j) = P(i,j) + D(i,j) - A(i,j) + A(j,i)$

The most advantageous sequence change can be found by evaluating

$E(i,j)$, $P(i,j)$ and $D(i,j)$ for

$(i = n-1, n-2, \dots, 2, 1)$ and

$(j = i+1, i+2, \dots, n)$.

and then choosing the largest positive value among these.

The exchange used by Rubin , $E(i,j)$, is in fact a simultaneous promotion, $P(i,j)$, and demotion, $D(i,j)$. Because he always does these together, the advantage of a promotion is often nullified by the disadvantage of the corresponding demotion and vice versa. By allowing promotion and demotion to be done individually, this can be overcome.

The priority of the changes used in the improved method is:

1. profitable exchange
2. profitable promotion
3. profitable demotion
4. least adverse exchange if no profitable modification exists.

In the event of equally advantageous changes, the last one encountered using the designated evaluation of E , P and D is used. The fourth priority is usually a null

improvement change (ie. no change in the number of recycle assumptions required.)

c. Randomization and Termination

After a number of sequence changes have been made a stage is reached when no improvement of the sequence can be found. At this point null improvement changes usually occur indefinitely. The useless continuation of the search is stopped after a specified number of such null improvement modifications have been made. A new initial sequence is produced using a random number generator. The search for the optimum sequence is re-begun using this randomized sequence. Although the optimum is usually achieved with the first application of the algorithm, this is not guaranteed since the method is empirical. After a specified number of sequence randomizations the optimization is discontinued.

The problems associated with Rubin's original method were effectively eliminated by the method modifications. The true optimum of every example tried, was achieved and was invariably reached quickly. The example cited by Rubin as being unsolvable by his method was easily solved using the modified method. If this success gives a meaningful indication, the developed method is most satisfactory for optimization of calculation sequence.

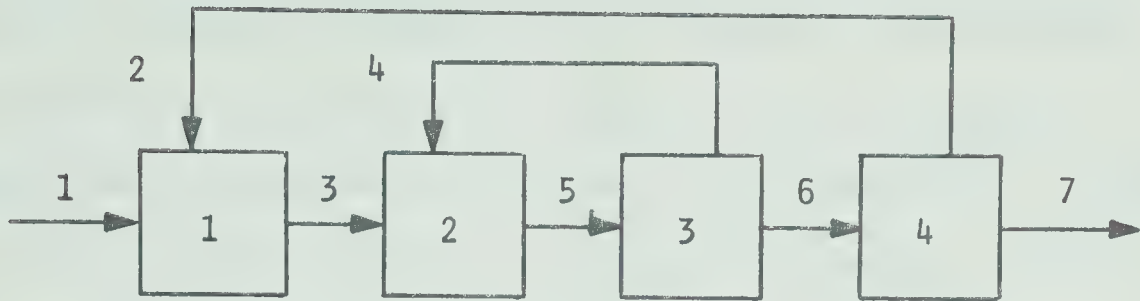
D. Executive Program

The executive program begins a design or simulation job by transferring control to a "sub-executive" data input module. Optimization of the calculation sequence to be used is normally done next. This is completed by a module utilizing the method described in the previous section. Optimization is not done if 'NO OPTIMIZATION' is specified in the data. In this case a user supplied calculation sequence is used (see Chapter V.).

The necessary process calculations are completed using the calculation sequence (optimized or specified). The executive calls the equipment modules in turn. As the calculations proceed, assumed quantities are stored by the executive. When new improved values are calculated, these are compared with the old ones to check for convergence. Recycling the calculations when required is achieved by merely changing the location in the calculation sequence.

Several recycling strategies may be adopted. Perhaps the simplest is to recycle whenever a previously assumed stream is calculated. Figure V. shows the results of this as strategy 1. It was felt this would result in an unnecessary amount of nested looping and could lead to convergence problems.

The strategy adopted was: recycle after a previously assumed stream has been calculated, but only if all



Strategy 1

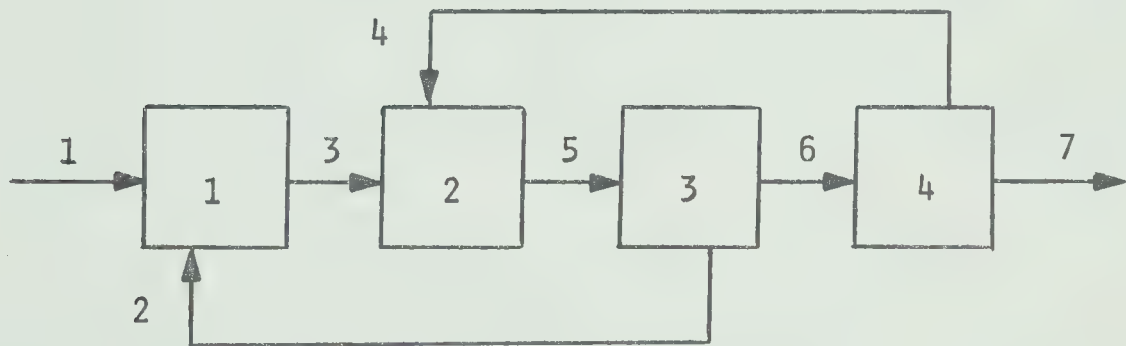
Calculation path: $\langle 1, (2-3, 2-3 \dots), 4 \rangle \langle 1, (2-3, 2-3 \dots), 4 \rangle \dots$

Convergence of stream $S(4)$ obtained for each estimate of $S(2)$.

Strategy 2

Calculation path: $\langle 1-2-3-4 \rangle \langle 1-2-3-4 \rangle \dots$

Convergence of streams $S(2)$ and $S(4)$ obtained simultaneously.



Strategy 1

Calculation path: $\langle (1-2-3, 1-2-3 \dots), 4 \rangle \langle (2-3, 1-2-3 \dots), 4 \rangle \dots$

Convergence of stream $S(2)$ obtained for each estimate of $S(4)$.

Strategy 2

Calculation path: $\langle 1-2-3-4 \rangle \langle 1-2-3-4 \rangle \dots$

Convergence of streams $S(2)$ and $S(4)$ obtained simultaneously.

FIG. V TWO RECYCLE CALCULATION STRATEGIES

previously assumed streams have been calculated. The results of this are shown in Figure V. as strategy 2.

When the process calculations are complete a process calculation summary module is called if a summary is desired (See Chapter V). This completes the job execution.

The executive developed is far more sophisticated than is necessary for sulphur plant process calculations. The sophistication is necessary to achieve the general applicability that was desired.

III. DETERMINATION OF EQUILIBRIUM COMPOSITIONS

During the process calculations, the determination of stream compositions entails more than material balances if chemical reactions are involved. Ideally the reaction compositions are found using chemical kinetics. However, in the sulphur plant application, this is presently impossible due to a lack of kinetic data. In many reaction systems not limited severely by kinetics, thermodynamic equilibrium is nearly achieved. For this type of system, the stream compositions predicted by a thermodynamic equilibrium approach become valid. It has been assumed that when proper reaction conditions exist, the sulphur recovery reactions achieve equilibrium. The determination of thermodynamic equilibrium compositions by free energy minimization will be described.

A. Minimization of Free Energy (M.F.E.)

There has been a considerable amount of work done on the efficient computation of complex equilibria (23,24,25,26,27,28,29), particularly in the field of rocketry. The "equilibrium constant" method has long been used for determining equilibria for simple reaction systems. This method uses algebraic equations, derived from stoichiometry, which take account of the reaction equilibrium constants. However, complex systems involve

large numbers of chemical reactions and molecular species which result in sizeable sets of highly non-linear equations. The solution of these equations by a method such as Newton-Raphson is very difficult. Convergence to the solution is invariably slow and often cannot be achieved even with good guesses.

A more recent method of determining complex equilibria involves minimization of the system free energy. Reaction stoichiometry is ignored. Since minimum free energy is a criterion of thermodynamic equilibrium, the location of the minimum is equivalent to finding the equilibrium composition. This approach is far less susceptible to convergence difficulties and will converge even with very poor initial guesses.

A comprehensive paper has been written by Zeleznik and Gordon(29), reviewing the thermodynamic principles involved in equilibrium calculations. The development and extensions of the two approaches mentioned, as well as their relative merits and use are discussed. They seem to favour the free energy approach.

White, Johnson and Dantzig(23) presented the original method utilizing free energy minimization. They described two alternate means of minimizing a derived objective function - one using Newton-Raphson steepest descent and the other, linear programming. The method developed was limited to gaseous equilibria but was later extended to multi-phase equilibria by Oliver, Stephanou and Baier(24).

The original method of Dantzig et al was considered adequate for the reaction systems encountered in sulphur recovery processes. The steepest descent procedure described by them was used for the free energy minimization. A brief derivation of this method follows.

The free energy of a mixture of n molecular species, containing $x(i)$ moles of the i th specie can be expressed as:

$$F(\underline{X}) = \sum_{i=1}^{i=n} f(i) \quad (1)$$

where $\underline{X} = x(1), x(2), \dots, x(n)$, the set of mole numbers,

$$f(i) = x(i) \cdot (c(i) + \ln \langle x(i)/X_B \rangle),$$

$$c(i) = F/RT(i) + \ln P,$$

P = the total pressure in atmospheres,

$$X_B = \sum_{i=1}^{i=n} x(i), \text{ and}$$

$F/RT(i)$ = the i th specie molal standard (Gibb's) free energy function.

The equilibrium composition is that non-negative set of mole numbers which minimizes (1), subject to the atomic mass balance constraints:

$$\sum_{i=1}^{i=n} a(i,j) \cdot x(i) = b(j), \quad (j=1, 2, \dots, m)$$

where m = the number of atomic species,

$a(i,j)$ = element of formula matrix, A , representing the number of atoms of the j th atomic specie associated with the i th molecular specie,

$b(j)$ = total number of j th specie atoms in system.

Starting with a positive set of values for the mole numbers, $\underline{Y} = y(1), y(2), \dots, y(n)$, satisfying the mass balance constraints, the free energy of the mixture is:

$$F(\underline{Y}) = \sum_{i=1}^{i=n} y(i) \cdot (c(i) + \ln \langle y(i)/Y_B \rangle)$$

Using a Taylor expansion about \underline{Y} and introducing Lagrangian multipliers, $(l(j), j=1, 2, \dots, m)$, to ensure that the mass balance constraints are satisfied, an approximation for \underline{X} is obtained:

$$x(i) = -f(i) + (y(i)/Y_B) + y(i) \cdot \sum_{j=1}^{j=m} l(j) \cdot a(i, j) \quad (2)$$

$$\text{where } f(i) = y(i) \cdot (c(i) + \ln(y(i)/Y_B)) \quad (3)$$

Summing over i ,

$$\sum_{j=1}^{j=m} l(j) \cdot b(j) = \sum_{i=1}^{i=n} f(i)$$

If the following constants are defined:

$$r(j, k) = r(k, j) = \sum_{i=1}^{i=n} a(i, j) \cdot a(i, k) \cdot y(i), \quad (j, k = 1, 2, \dots, m),$$

$$p(j) = \sum_{i=1}^{i=n} a(i, j) \cdot f(i), \quad (j = 1, 2, \dots, m),$$

$$q = \sum_{i=1}^{i=n} f(i), \text{ and}$$

$$u = X_B/Y_B - 1,$$

then a set of $m+1$ linear equations in the unknowns $l(1), l(2), \dots, l(m)$ and u results:

$$\begin{array}{rcl}
 r(1,1).l(1) + r(1,2).l(2) + \dots + r(1,m).l(m) + b(1).u & = & p(1) \\
 r(2,1).l(1) + r(2,2).l(2) + \dots + r(2,m).l(m) + b(2).u & = & p(2) \\
 \vdots & & \vdots \\
 r(m,1).l(1) + r(m,2).l(2) + \dots + r(m,m).l(m) + b(m).u & = & p(m) \\
 b(1).l(1) + b(2).l(2) + \dots + b(m).l(m) + 0 & = & q
 \end{array}$$

The solution of these equations (by Gaussian elimination) yields $l(j)$, the Lagrangian multipliers. Substitution of these multipliers and the results of Equation (3) into Equation (2) produces a new approximation, \underline{X} , to the equilibrium mole numbers. This procedure is repeated until convergence is achieved.

If the procedure described is unconstrained, some mole numbers may become negative. Since this is impossible physically, it is unacceptable. To prevent negative mole numbers, the following procedure is used:

1. the computed changes are found,

$$d(i) = x(i) - y(i) ,$$

2. the limiting change is found,

$$S = \min. \text{ abs. } y(i)/d(i), \text{ over all non-positive } x(i)\text{'s},$$

$$S = 1 \text{ if all } x(i)\text{'s are positive,}$$

3. new approximations are defined,

$$x(i)' = y(i) + S.F.d(i) .$$

Due to the nature of Lagrangian multipliers, the mass balance constraints are satisfied for any value of F (or

S.F). Therefore, the value of F may be adjusted to render all mole numbers positive. For $F=1$, the limiting specie (ie. specie defining S) is set to zero. This is undesirable because of the nature of Equation (2). Once a molecular specie becomes zero it remains zero interminably. Dantzig et al attempt to optimize the selection of F , but this was not done in the present application. Rather, a constant value $F = 0.99$, was chosen as done by Oliver et al. This is found satisfactory, as it limits a specie reduction to 99 percent (one hundred fold reduction) of its previous value.

B. Implementation of the M.F.E. Method

The free energy minimization method was programmed and tested using several literature examples (23,24), and identical results were obtained. The use of the program for other applications, however, resulted in several difficulties.

The first of these was the determination of an initial positive (non-negative, non-zero) set of mole numbers. Frequently, some of the mole numbers in the specified feed (particularly reaction product species) are zero. As stated previously, the method will not alter mole numbers which are identically zero. The generation of an initial positive set of mole numbers, rigorously satisfying the mass balance constraints is not trivial in this case. The number of

molecular species is invariably greater than the number of atomic species and this results in more unknown mole numbers than mass balance equations. Arbitrary specification of the excess unknowns does not guarantee the remaining ones will be positive.

Several means of resolving this problem were tried. The only method found which generated a positive set rigorously satisfying the mass balance constraints was a modification of the simplex (linear programming) algorithm. Unfortunately, finding the initial positive set took much longer than the free energy minimization itself. It was decided in the interests of saving the time and space required by the simplex algorithm, that species initially zero would be equated to an arbitrarily small number (say 10^{-6}). This introduces small errors into the mass balances but results in a negligible difference in the equilibrium compositions. Convergence takes longer because of the very poor guesses, but is always achieved due to the excellent convergence characteristics of the method. Obtaining an initial positive set in this way was found to be completely satisfactory.

The safeguards taken to prevent negative or prematurely zero mole numbers sometimes impede convergence. This is because species tending to zero are limited to a one hundred fold decrease. Non-zero species are prevented from becoming zero but convergence of zero species is considerably slowed. Furthermore, while species not present are decreasing to

zero, the minimization is effectively suspended, due to the negligible changes being imposed. For example, the composition may remain essentially constant for 30 iterations while one specie is driven from 10^{-10} moles to a stable value of 10^{-70} moles. The minimization then continues until a similar situation is encountered or until convergence is achieved. This convergence impairment can be partly eliminated if species less than some criterion (say 10^{-10}) are equated to zero. The choice of the criterion is quite critical. Some species (particularly those initialized to 10^{-6}) decrease before obtaining their final equilibrium value. If this value should be positive, it is imperative that the mole number not be equated to zero during the minimization, as this will result in an invalid equilibrium composition. The choice of 10^{-10} is a compromise between waste of computer time and risk of an invalid composition. If the latter is suspected, the calculations can be repeated using a positive set derived from the "equilibrium composition". If the composition is valid, it should be reproduced.

The paramount importance of including all molecular species that might exist and positive initial mole numbers for them should be emphasized. Species which are thermodynamically precluded at equilibrium will be driven to zero during the minimization. However, species not included or initially zero cannot possibly have a final positive value. If a significant specie is so omitted, an invalid

composition will result.

It is useful to realize that if a "good" initial guess exists, the generation of a positive set of mole numbers may be unnecessary. If species which are initially zero are known to be nonexistent at equilibrium, a considerable time saving results from skipping the positive set generation. Convergence is then faster because fewer species must be driven to zero.

C. Application of the M.F.E. Method

The adapted method, when programmed, was found to be satisfactory for all the examples tried. The program was then generalized to accommodate any reaction system, as defined by a feed composition. Any molecular specie may be included in the feed (with a mole number of zero) as a possible product. Those species which are physically impossible (eg. COS in an H O S N system) are eliminated during initialization and ignored thereafter. Program generation of an initial positive set of the remaining mole numbers may be specified or skipped. Species which are non-existent at equilibrium will be driven to zero (10^{-10}) during the free energy minimization. The program generalization was necessary to accommodate the variation of atomic species present in the different plant streams; all compositions were to be calculated using the same equilibrium program and the same thermodynamic property

data.

An example of the use of the composition calculation module as an independent program is illustrated in Figure VI. The variation of equilibrium mole fractions with temperature has been plotted for a typical sulphur plant feed composition.

Reaction Quenching and Sulphur Shift

An important restriction must be imposed on the calculations for the sulphur recovery reactions. At high temperatures (above 1000 F), the reactions take place homogeneously and thermodynamic equilibrium is approached. However, at low temperatures, total equilibrium is approached only in the presence of a catalyst. In the absence of a catalyst, essentially no reaction takes place; only the distribution of sulphur among the elemental sulphur species changes. This sulphur shift occurs at all temperatures. Therefore, in Figure VI, at temperatures below 1000 F, the presence of a catalyst has been assumed, since the equilibrium compositions have been plotted.

Thermodynamic equilibrium compositions are independent of the presence of a catalyst. This is because catalysis is a kinetics phenomena. Thermodynamic equilibrium represents the limiting reaction condition, while kinetics is related to the rate at which this condition is approached. Even though kinetics are not dealt with directly in the calculations, some account must be taken of severely

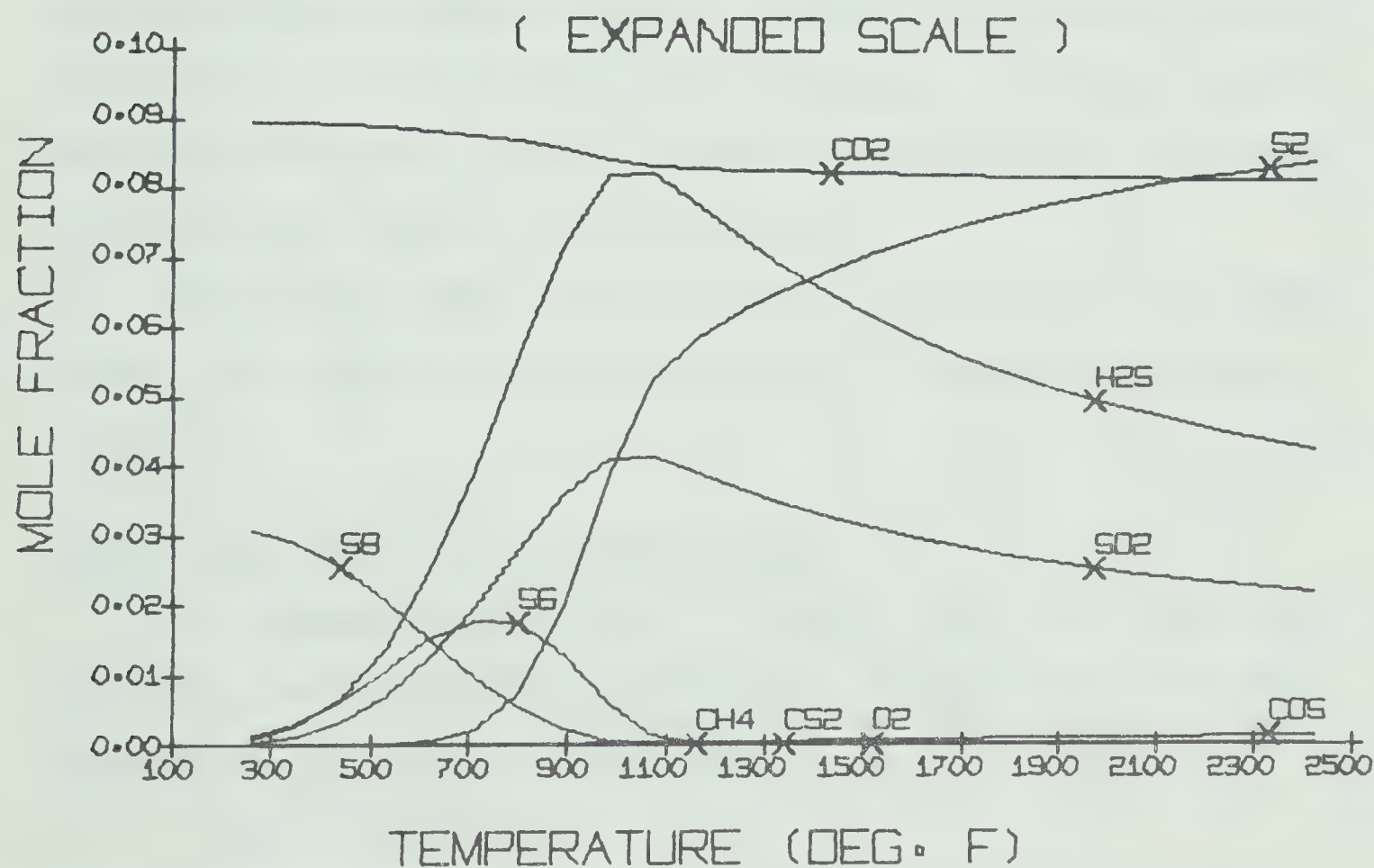
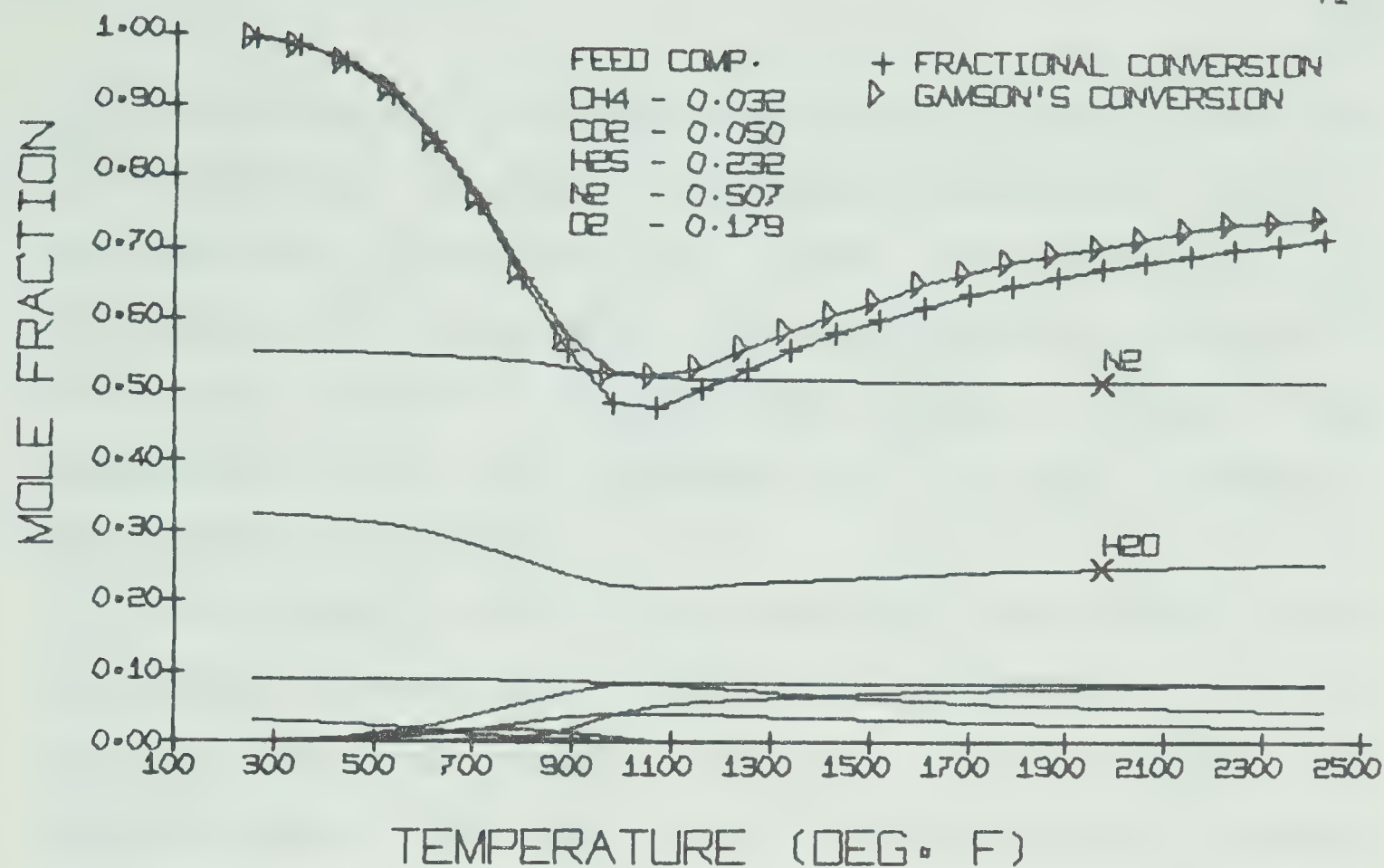


FIG. VI EFFECT OF TEMPERATURE ON COMPOSITION AND CONVERSION

limiting kinetics if realistic results at all conditions are to be obtained. An "equilibrium cutoff temperature" concept has been used to achieve this. Below this temperature, in the absence of a catalyst, all reactions but the sulphur shift are assumed to be completely quenched. Above this temperature or in the presence of a catalyst, complete equilibrium is assumed.

The sulphur shift is simulated (at temperatures below the cutoff temperature) by extracting the elemental sulphur species from the real stream and placing them in a pseudo-stream. The equilibrium distribution of sulphur species in the pseudo-stream is calculated at the specified temperature and sulphur partial pressure of the real stream. Iteration is required due to the change in sulphur partial pressure produced by the sulphur redistribution. The real and pseudo-streams are then combined.

Conditions when equilibrium is calculated and when kinetic limitations are artificially imposed are shown in Table I.

Iterative Temperature Determination

The composition module is also used for obtaining adiabatic and non-adiabatic reaction temperatures. The heat balance for a reacting stream is:

$$H(1) = H(2) + Q ,$$

where the functions of temperature are:

$$H(1) = \text{the inlet stream enthalpy (a function of}$$

TEMPERATURE AND/OR STREAM CONDITION	EQUILIBRIUM CUTOFF TEMPERATURE	COMPOSITION CALCULATION METHOD
<ul style="list-style-type: none"> - temperature within homogeneous reaction range, - temperature greater than cutoff temperature, - no catalyst present 	greater than 1000 degrees fahrenheit	<ul style="list-style-type: none"> - complete thermodynamic equilibrium calculated at specified temperature
<ul style="list-style-type: none"> - stream cooled from homogeneous to catalytic reaction range, - temperature less than cutoff temperature, - no catalyst present 	(ie. lower limit of homogeneous reaction range)	<ul style="list-style-type: none"> - complete thermodynamic equilibrium calculated at cutoff temperature, - sulphur shift done on cutoff composition at specified temperature
<ul style="list-style-type: none"> - temperature in catalytic reaction range, - temperature greater than cutoff temperature, - no catalyst present 	less than 400 degrees farhenheit (ie. lower limit of catalytic reaction range)	<ul style="list-style-type: none"> - complete thermodynamic equilibrium calculated at specified temperature
<ul style="list-style-type: none"> - temperature in catalytic reaction range, - no catalyst present 	negative and purely a flag	<ul style="list-style-type: none"> - sulphur shift done on given composition at specified temperature

TABLE I. RELATION OF COMPOSITION CALCULATION TO STREAM CONDITION

inlet composition and temperature),
 $H(2)$ = the outlet stream enthalpy (a function of the
 unknown outlet temperature and composition),
 Q = stream heat loss (zero for adiabatic case).

The problem is to find the final temperature ($T(2)$) which satisfies the heat balance. If enthalpy was a function only of temperature, this would be quite simple. However, enthalpy is a strong function of composition which in turn is a moderate function of temperature. The determination of the outlet temperature therefore involves iterative guessing. At each temperature, the equilibrium composition and heat loss, if any, are calculated and the resulting heat balance error is evaluated. Convergence has been achieved using the secant method. After two initial guesses have been made, succeeding approximations to the correct temperature are obtained as follows:

$$T(i+1) = T(i-1) - A \cdot (T(i-1) - T(i)) \cdot E(i-1) / (E(i-1) - E(i))$$

where $T(i+1)$, $T(i)$ and $T(i-1)$ are the new, present and old
 outlet temperature guesses respectively,

$$\begin{aligned} E(i) &= H(1) - H(2) - Q \quad (\text{heat balance error}) \\ &= H(1) - H(2) \quad \text{for adiabatic case, and} \end{aligned}$$

A = a convergence accelerator (usually set to 1.0
 if no convergence problems exist).

Iteration on the outlet temperature is discontinued when the relative error,

$$ER(i) = \text{abs. } E(i) / H(1) ,$$

is less than some predetermined criterion.

Since each temperature guess involves an iterative calculation of the equilibrium composition, it can be seen that determination of adiabatic and non-adiabatic temperatures involves a large amount of computation. This can be reduced by skipping the positive set initializations (during composition calculations) when the correct temperature is approached.

D. Thermodynamic Data Sources

Improved convergence characteristics is not the only aspect of free energy minimization that is superior to the equilibrium constant method. Another significant advantage is that no account of reaction stoichiometry must be taken. This greatly assists the generalization of a program utilizing the method, since "reaction bookkeeping" is eliminated. To complete the composition calculations, only the molecular specie free energy functions are required. Similar functional forms are required for enthalpy evaluations. However, if stoichiometry is to be ignored, these functions must be in a particular form. Both free energy and enthalpy must be functions of temperature relative to a common reference. If this is so, the functions include both chemical and sensible energies. Therefore, the changes in free energy and enthalpy with reaction are automatically accounted for and need not be calculated separately. Most thermodynamic data sources use

many bases and, to ignore stoichiometry, this data must be converted to a common base.

Thermodynamic property data in tabular or functional form may be obtained from several sources (30,31,32,33). A comprehensive listing of sources has been detailed (34).

For the sulphur plant application, a particularly good source of thermodynamic data was the NASA "Thermodynamic Properties to 6000 K for 210 Substances Involving the First 18 Elements"(30). This data, accumulated for rocket studies, is very well suited to the present needs. Besides a tabular presentation, functional constants are given for thermodynamic properties including F/RT , C_p/R , H/RT and S/R . This data is referenced to a common base and so may be used directly. Most of the molecular species encountered in sulphur recovery are available from this source. The notable exceptions are S(6) and S(8) forms of elemental sulphur and hydrocarbons excluding methane. Kelley(35) has presented functions for free energy changes for S(2) to S(8) and for S(2) to S(6). Since S(2) was included in the NASA presentation, constants compatible with the NASA form were derived for S(6) and S(8). No other forms of elemental sulphur were included, although some data on these has been presented (36). Except for methane, no hydrocarbon data in the derived form was found. Existing hydrocarbon data, referenced to many bases, may be converted from other sources to a form compatible with the NASA source by curve fitting. This data conversion has not been done here.

IV. EQUIPMENT MODULES

As stated previously, the equipment modules are independent programs, but must be compatible with the executive program. In particular, the compatibility of data accessing and storing by the modules is essential. Of lesser importance is a compatible form of output. Data is stored primarily in a program 'common' area and is manipulated entirely by the modules and not by the executive. Data input, data storage and output of results are described in detail in Chapter V.

During the process calculations, the executive repeatedly decides which equipment number is to be done next. The streams to and from this equipment are found and the area of data storage allotted to that equipment number is defined. An output priority flag (see Chapter V.) is set for the process calculations to follow. Finally, the equipment type is determined and program control is transferred to the appropriate equipment module.

The process calculations involve three types of streams. These are defined as follows:

1. conventional material streams which involve mass and energy flow and associated physical properties (eg. most process streams),
2. service streams which are identical to material streams but are ignored during the calculation optimization (eg. boiler feedwater and steam, furnace fuel etc.), and,

3. information streams which have only information associated with them, and are frequently opposite in direction to material stream flow (eg. stream split ratio, energy transfer etc.)

The modules which are developed must be programmed to accommodate the presence or absence of these stream types.

Several "executive type function" routines have been included which are not directly related to the executive, but which can be used by the modules when required. These include stream utility routines and data compatibility checking etc.

Nine equipment modules have been developed for the sulphur plant application. Each of these is capable of functioning in either a design or a simulation mode, as determined by the data accessed. These are:

- | | |
|---|---------|
| 1. reaction furnace and waste heat boiler | (RXWHB) |
| 2. in-line burner | (INLNB) |
| 3. catalytic sulphur converter | (CNVTR) |
| 4. sulphur condenser | (CONDR) |
| 5. adiabatic stream combiner | (COMBN) |
| 6. stream combiner and/or divider | (CMBDV) |
| 7. combustion air adder | (AIRAD) |
| 8. tail gas incinerator | (INCIN) |
| 9. effluent stack | (STACK) |

These modules can be used to design or simulate a large variety of sulphur plants, but will not accommodate all possible flowsheets. To do this would require several more

special purpose modules. The distinct parts of the modules which have been developed will be described individually.

1. Reaction Furnace and Waste Heat Boiler

The most complex module that has been developed is the reaction furnace - waste-heat boiler. The complexity arises from the large number of boiler designs and options that are used in sulphur recovery plants. The purpose of the reaction-boiler is to burn some of the feed hydrogen sulphide and hydrocarbons with the air supplied. The combusted gas is then cooled from the flame temperature (about 2000 F) to a significantly lower temperature.

The module developed will accommodate a large variety of boilers, but not all industrially used boilers. To begin with, only fire-tube boilers can be handled. The calculation of heat losses (particularly radiative) are much simpler for this type of boiler than for the alternate water-tube type. The accommodation of the latter would entail development of additional and entirely different convective and radiative heat loss routines.

The combustion may be done using either a muffle furnace or a boiler fire-tunnel. A muffle furnace is an insulated reaction chamber external to the boiler. Combustion of the acid gas takes place adiabatically and a multi-tube first pass is used in the adjoining boiler. A boiler fire-tunnel is a single large diameter tube which

forms the first pass of the boiler. In this case, some heat transfer occurs during combustion and so the reaction is non-adiabatic. For either type of combustion chamber, the boiler section of the equipment may consist of one, two or three tube passes.

The design of the boiler combustion chamber is identical to that used for the in-line burner, and will be described with that equipment module. It has been assumed that thermodynamic equilibrium is achieved in the combustion chamber if sufficient residence time (eg. 0.6 sec.) is provided. This is because the high temperatures reached during combustion are accompanied by very rapid kinetics. However, as the cooling in the boiler takes place, the combustion reactions reverse and the reaction rates decrease. Since no catalyst is present, the reactions are quenched as the temperature decreases. Industrially it has been found that the boiler exit composition and hence sulphur conversion (at say 600 F) resembles the equilibrium prediction at a higher temperature. The quenching responsible for this is simulated by using an equilibrium cutoff temperature (say 1100 F) that produces a realistic outlet stream. Below the cutoff temperature, only the sulphur shift reactions occur.

Another boiler option that has been implemented is the use of boiler bypass for process reheating. If bypass is used, one, two or three boiler bypass reheat streams may exist. Whereas in reality the bypass is a single stream,

calculationally it is divided within the boiler into the number of reheat streams required. The bypass is always extracted at the exit of the second last tube pass, regardless of the number of boiler passes. The reheat streams are found by successively multiplying the remaining boiler stream by a split fraction (bypass ratio). The residual gas then passes through the last boiler pass.

Boiler Tube Pass Design

Valdes(37) has presented a paper for the design of firetube reactor-wasteheat boilers, with special reference to sulphur plants. This method was not considered sufficiently rigorous since it was assumed that composition was constant throughout the boiler. The enthalpy changes accompanying chemical reaction during cooling have been found to be significant and so are not ignored in this work. Although the approach proposed by Valdes was not used, his work provided a useful reference for heat transfer and pressure drop calculations.

The design variables associated with each tube pass are tube length, tube diameter and the number of tubes. In the present method of design, the tube length must be specified if a muffle furnace is used. If a boiler firetube is used, the design of the first pass firetube will define the boiler tube length. In either case, the choice of length (same for all passes) is limited by commercial availability.

For each boiler tube pass the maximum allowable

pressure drop and the outlet temperature are specified. The number of tubes and the tube diameter which satisfy these specifications must be found. This is done by iteratively guessing the tube number. For each guess, a commercially available diameter which results in less than the specified maximum pressure drop is found. The resulting heat loss is then calculated. Since the outlet temperature is specified, the outlet composition must be calculated only once. The secant method is used to find the number of tubes which results in the specified tube pass outlet temperature.

The discrete nature of the tube diameters (commercial) adversely affects convergence to the correct tube number. This is particularly true when the tube diameter alternates between two sizes with succeeding tube number guesses. Convergence is improved by the following strategy:

1. the two initial guesses required for the secant method are made significantly different,
2. a convergence accelerator less than one is used until the correct tube number is roughly approximated,
3. the tube diameter is fixed at the current value if a specified number of tube number iterations has been exceeded.

The tube number is rounded to the nearest integer number of tubes once it and the corresponding tube diameter have been determined. The outlet temperature is usually within a degree of that specified and the pressure drop is somewhat below the maximum specified.

After each tube pass design, the tube pass is simulated. This is done because simulation results are continuous (temperature and pressure) whereas design results (diameter and tube number) are discrete. The specified tube pass outlet conditions cannot be met exactly; simulation results in the actual outlet conditions for the designed pass.

Sometimes specification of all tube pass outlet temperatures is not desired. In this event "multiple tube pass design" is done. The intermediate tube pass outlet temperatures are estimated and it is temporarily assumed that the tube passes involved are identical. This type of design is subject to all outlet (including bypass) temperatures being specified. The "multiple design" should be elucidated by the following calculation sequence for a three pass boiler (no bypass) with all pressure drops and only the final exit temperature specified:

1. define first pass design to satisfy outlet specifications on basis that all three passes are identical - estimate first and second pass exit temperatures,
2. simulate first pass,
3. define second pass on the basis that second and third passes are identical - estimate second pass temperature,
4. simulate second pass,
5. define third pass to satisfy the outlet temperature and final pass pressure drop specifications,

6. simulate third pass.

The repeated design of the last two passes is necessary because of the approximate nature of the initial designs; averaged stream compositions and properties over a large temperature interval are used.

Boiler Tube Pass Simulation

Tube diameter, tube length and number of tubes must be specified for each pass when boiler simulation is being done. The simulation of each pass involves a non-adiabatic temperature determination. At each estimate of outlet temperature, the resulting composition, heat loss and pressure drops are calculated. Iteration on the temperature continues until the tube pass energy balance is satisfied.

The total heat loss in the boiler consists of convective and radiative heat transfer. The latter is of primary significance at high temperatures. Below 900 F (mean tube pass temperature) radiation is assumed to be negligible. The method used by Valdes to evaluate convective heat losses has been used, but his method of calculating radiation heat losses using graphical emissivity data has not been used. It is desirable to avoid tabular interpolation or graphical data.

Radiation heat losses are difficult to evaluate rigorously because of the effect of physical geometry and the problem of obtaining emissivities. For simple geometries, a radiating beam length is used to account for

physical structure. In the present case the beam length used is 0.9 times the tube diameter. Empirical correlations for emissivity data as a function of temperature, pressure and composition are nearly non-existent. The best source of emissivity data for the present needs was found in Hottel(38). Emissivity data previously obtained for water carbon-dioxide mixtures is represented with a single curve. The product of the sum of water and carbon dioxide partial pressures is plotted against the product of gaseous emissivity and absolute temperature. Several points along the nearly linear plot presented by Hottel have been used to find emissivities by linear interpolation. It has been assumed that sulphur dioxide resembles carbon dioxide and hydrogen sulphide resembles water in this context. The partial pressure used to evaluate the emissivity is the sum of the partial pressures of all polar molecules (molecules with three or more atoms are assumed to be polar).

The equation presented by Valdes to evaluate pressure drops in the tubes, including end effects, has been used. His graphical determination of friction factor has been replaced with an empirical correlation.

The equations pertaining to the calculation of convective and radiative heat transfer, pressure drops and steam production for a specified boiler steam pressure are presented in Appendix A.1. A list of the specifications required for various boiler designs or simulations and a list of boiler equipment parameters are to be found in

Appendix B.

2. In-line Burner

The in-line burner is used for the combustion of a small percentage (eg. 5 percent) of the acid gas feed with the stoichiometric amount of air. The resulting hot combusted gas is used for process reheating by combining it with the stream entering a converter. In reality the burning and stream combining take place in a single equipment unit. However, from a calculation standpoint, the burning alone takes place in the in-line burner. The in-line burner is then invariably coupled with an "adiabatic stream combiner" where the two streams are combined and a sulphur shift is done.

It has been assumed that the hot gas is instantly quenched by the large volume of cooler gas. Therefore the reversal of the combustion reactions that occurs in the boiler does not take place in the in-line burner.

Combustion Chambers

The combustion chamber aspects of the in-line burner, the muffle furnace, and the boiler fire-tube are handled in exactly the same manner. The following therefore applies equally to all three types of combustion chambers. Concern is centered only on a characteristic length and diameter for the chambers and on the resulting unit volume heat release

and the combustion chamber residence time. A detailed mechanical design of the burners etc. is not done and neither is an analysis of the flame stability (or flame combustion mechanism) done. Such an analysis, as done by Fristrom(39), requires more data than is presently available for the sulphur system.

The first step of either the simulation or the design case is determining the adiabatic flame temperature. In practise, if this temperature is not sufficiently high, difficulties in maintaining a stable flame will be encountered.

Combustion Chamber Design

In the design case, a maximum allowable heat release (per unit volume) and/or a minimum residence time within the combustion chamber may be specified (eg. 0.6 sec. residence time and/or 50,000 BTU/hr. cu. ft. heat release). The minimum volume required to satisfy the specification(s) must be found. From a selection of commercially available tube lengths and diameters, a length and diameter yielding a volume at least as large as that required are found. Furthermore the length to diameter ratio is chosen as close to 4:1 as possible. The actual residence time and heat release are then found by simulation.

Combustion Chamber Simulation

For combustion chamber simulation, the effective chamber length and diameter must be specified. Once the

adiabatic flame temperature is determined, the unit volume heat release is calculated. Stoichiometry and heats of reaction are not involved in this calculation; the total heat release is defined here to be the difference between the enthalpy of the reaction products at the flame temperature and at the inlet temperature. The unit heat release is found by dividing the total heat release by the combustion chamber volume. The combustion residence time is based on ideal gas behaviour. The volumetric flow rate of inlet gas at the flame temperature is divided by the chamber volume to yield the residence time. (See Appendix A.1 and B.)

3. Catalytic Sulphur Converter

The primary purpose of the converter is to catalytically react hydrogen sulphide and sulphur dioxide (usually in the ratio 2:1) to form elemental sulphur and water. It is also desirable to convert other non-elemental forms of sulphur (eg. carbonyl sulphide and carbon disulphide) to elemental sulphur, but this is not always achieved in commercial units. The converters are operated within the catalytic temperature range of the reactions involved, since in this region high equilibrium conversions are possible. The important design and operating considerations are:

1. equilibrium conversion for the primary reaction

- increases with decreasing temperature, so it is desirable to operate the converter at low temperatures,
2. kinetics decrease with decreasing temperature, so at sufficiently low temperatures (below 425 F), equilibrium will not be approached due to kinetic limitations,
 3. condensing sulphur within the converter will foul the catalyst and so all points within the converter must be above the sulphur dew point,
 4. sufficient residence time must be provided in the converter for equilibrium to be kinetically approached.

Sometimes the first converter is operated at a higher temperature to eliminate the carbonyl sulphide. This is not always successful. In contrast to the primary reaction, the conversion of carbonyl sulphide to sulphur should increase with temperature from both kinetic and thermodynamic standpoints.

Converter Design

Since the relevant kinetic data is not available, some other means of designing the converter must be used. Industrially, even though converter bed temperature rises may occur entirely within the first few inches, the catalyst beds are invariably three feet or more thick. This is partly to compensate for deactivation of the catalyst with time.

The converter design consists of determining the

required bed thickness and cross-sectional area, using empirical criteria and assuming ideal gas behaviour. As common practise dictates, the cross-sectional area is defined by a specified maximum allowable lineal gas velocity (eg. 1 foot per second) through the bed. The minimum converter volume is set by a flowrate criterion (eg. 3. pound moles (or 1000 standard cubic feet) per hour per cubic foot of catalyst bed). Provided it is greater than 3 feet, the bed depth is found by dividing the minimum volume by the cross-sectional area.

Converter Simulation

The lineal gas velocity and molal flow rate resulting from the specified bed depth and cross-sectional area are calculated during converter simulation. For both simulation and design the converter outlet temperature and equilibrium composition are found by an adiabatic temperature determination. The pressure drop through the catalyst bed is estimated using an empirical correlation.

Once the outlet temperature has been found, the converter temperature rise is divided into several temperature intervals. At the end of each interval the sulphur dew point is calculated to check that it is (25 F) above the converter bed temperature. This is done on the basis that conversion is proportional to the temperature rise. If the dew point is too low, the converter inlet should be increased or sulphur condensation will occur

within the catalyst bed.

The equations for converter simulation and design are presented in Appendix A.3.

4. Sulphur Condenser

The rigorous calculation of partial sulphur condensation is very difficult. The complexities of partial condensing are compounded by the mass transfer limitations resulting in fog formation. An attempt has been made to calculate the heat transfer, sulphur condensation and fog formation occurring in the sulphur condenser. The common practise of using an empirical, constant value for the overall heat transfer coefficient was considered inadequate.

Calculational procedures for designing cooler condensers, including partial condensation applications, have been described by Ludwig(40) among others(41,42). Ludwig's approach treats a partial condenser with a superheated gas-vapour inlet as two distinct units - a desuperheating cooler and a saturated vapour condenser. This technique is frequently used and reportedly results in overdesign. The formation of fog is precluded in the analysis since after desuperheating, the gas-vapour mixture is assumed to always be at saturated conditions.

An analog computer method of designing cooler-condensers with fog formation has been presented by Coughanour and Stensholt(43). Their method "generates" fog

to relieve super-saturations in the bulk gas if this should occur due to mass transfer limitations. Johnstone, Kelley and McKinley(44) have shown that bulk super-saturation is not necessary to form fog. They have presented a means of determining when cooler-condenser fog formation is theoretically possible from a thermodynamic standpoint under given condensation conditions. Their analysis takes into account radial variations of the gas-vapour mixture within the tubes but the results of the analysis are qualitative (ie. existence or absence of fog).

A combination of the work mentioned has been used for the present calculations. The gas-vapour mixture is not desuperheated in a preliminary section. Desuperheating occurs as condensation and cooling proceed. The rate of sulphur condensation on the tube walls is found to be mass transfer limited. If the bulk gas becomes super-saturated, it is assumed that fog is formed until saturation is reached; the supercooled mixture should be unstable in an industrial condenser. This is similar to the technique employed by Coughanour and Stensholt.

The method used predicts fog formation to relieve super-saturation but does not account for fog formed at or below saturation in the bulk gas. The radial variations of the gas within the tubes are ignored. Also it must be assumed that no entrainment of the sulphur condensate film occurs and that the fog does not conglomerate with the film. No account is taken of the reduction of fog by exit baffles,

the tube header or knock-out pots, if present. Because of the unknown magnitude of these effects, as well as the lack of reliable estimates of actual fog formation in industrial condensers, the qualitative validity of the method is unknown. The overall heat transfer coefficients calculated do tend to agree approximately with those used in commercial design.

Because of the large variations of stream conditions down the tubes, the condenser is analyzed in segments defined by temperature intervals. The lengths of the segments are unknown. Averaged stream properties are used for each segment and a sulphur shift is done at succeeding segment outlets.

The analysis of a condenser segment begins with finding the sulphur condensate film temperature for the segment. This temperature must be iteratively guessed to satisfy the energy balance on the segment condensate film. The energy transferred from the bulk gas to the film by heat and mass transfer must equal the heat transferred to the evaporating steam. This energy balance is presented in Appendix A.4 together with the other equations used in the method.

Once the condensate temperature satisfying the film energy balance is found, it remains to determine the segment length. If the number of tubes and the tube diameter have been defined, the segment heat and mass transfer area becomes a function of length alone. The length must be iteratively chosen to satisfy an energy balance on the whole

segment. The heat transfer to the steam is calculated for the guessed length. This must agree with the enthalpy changes of the tube-side segment streams. The segment bulk gas inlet and outlet temperature are known as they define the segment. The mass of sulphur transferred to the condensate film is a function of the length, and if the bulk gas is super-saturated at the segment outlet temperature, additional sulphur is condensed as fog. The present condensate temperature and the previous segment film temperature have been found. The correct segment length results in no energy balance error over the segment.

This procedure is used repeatedly for each condenser segment until the end of the condenser is reached. For the design case, where a specified maximum allowable mass velocity through the tubes dictates the number of tubes, termination occurs when the specified outlet temperature is reached. This temperature may be specified indirectly by specifying the desired percentage of inlet sulphur to be condensed (as fog and/or film). Simulation requires specification of tube diameter (as for design), tube length and the number of tubes. The calculations are discontinued when the specified length is achieved.

Because of the approximate nature of the fog calculations, the module allows for specification of the condenser outlet fog (pounds sulphur fog per hundred moles of inert gas). Below certain levels of outlet fog, defogging equipment is assumed to be present (ie. demister

pads or a coalescer.)

5. Adiabatic Stream Combiner

The adiabatic stream combiner does not correspond to any physical piece of equipment. It has been included to facilitate process stream reheating before catalytic conversion. The module combines a hot and a cold stream and finds the resulting outlet temperature. The calculation is done adiabatically, with a sulphur shift being the only allowed reaction. All other reactions are assumed to be instantaneously quenched when the hot gas is cooled by the larger cold gas stream.

The module has been programmed to accommodate the optional existence of an information feed-back stream. This option may be used to control the adiabatic stream combiner outlet temperature. If an output information stream exists, a routine is used to predict what the stream split, at the source of the hot gas, should be to yield the desired combiner outlet temperature. This prediction pertains to either the split between the boiler and the in-line burner or a boiler bypass split, and is conveyed to the appropriate equipment via the information stream.

The split required to achieve the desired outlet temperature is found iteratively. For each estimate, the effects on both the hot and the cold stream flowrates are evaluated. Then the resulting sulphur shift and outlet

temperature are found. Iteration using the secant method continues until the desired temperature results. The specified temperature and corresponding composition are used as the combiner outlet rather than the results of the initial split. This is so that equipment calculations following the combiner are realistic.

The option described is used in the design case where the combiner outlet (converter inlet) is specified. The prediction is done to reduce the recycle of process calculations. On the second pass of process calculations, the split(s) used (previously predicted on the first pass) will result in the desired combiner outlet temperature(s). For the simulation case, all stream splits are specified rather than guessed and so calculation recycle and information feed-back are unnecessary.

6. Stream Combiner and/or Divider

The stream combiner/divider is the most simple module developed. This module may be used to combine two or more streams and find the resulting temperature and pressure. No reaction of any type occurs. The stream combining is done by a stream utility routine which is also used for combining multiple feeds to other types of equipment. The pressure of the mixture is equated to the lowest non-zero feed pressure and the combined enthalpy is used to find the resultant temperature. Newton's method, utilizing heat capacity, is

used to converge to the correct temperature.

The inlet stream(s) may be divided into two outlet streams. A stream designation and split fraction defines the allocation to the outlet streams. The module will accept input of the stream split fraction via an information stream. If only a single output stream exists, the total input is directed to this outlet stream.

7. Combustion Air Adder

The combustion air adder is only a computational unit and does not exist as a physical piece of sulphur plant equipment. The module may be used at the point(s) where air is added for the combustion of acid gas. Given an acid gas inlet stream, the air required to complete the specified combustion is calculated and the necessary inlet air stream is created.

The fraction of non-elemental inlet sulphur to be completely oxidized may be specified (eg. 1 for 2/3 bypass plant boiler and 1/3 for straight through boiler). If this fraction is less than one, all non-elemental sulphur is assumed to be in hydrogen sulphide form. Oxygen requirements are calculated for the specified oxidation of carbon, hydrogen and sulphur. The nitrogen and water (relative humidity specified) accompanying this oxygen are found and added to the oxygen to form the inlet air stream.

When the air stream has been defined, it is combined

with the acid gas feed stream and the resulting temperature and pressure are found. The combined stream becomes the equipment outlet.

This module is intended for design purposes, where only the acid gas feed is specified. In the simulation case, or where both the acid gas and air streams are known and specified, the two should be fed to the appropriate equipment either as separate streams or as a combined stream. There is no need to use a combustion air adder if the air stream is specified.

8. Tail Gas Incinerator

Before the tail gas is vented to atmosphere via the stack it is incinerated to increase the stack exit temperature and to oxidize all forms of sulphur to sulphur dioxide. The incineration is achieved by adding a fuel gas (usually sweet gas) and air to the exiting process stream and then igniting the mixture. Excess air is generally introduced to the incinerator to ensure complete combustion.

Incinerator Design

For the design case an incinerator outlet temperature is specified. A small fuel gas stream is given to indicate the composition of the fuel gas. The ratios of specified to stoichiometric air to be used for combustion of the fuel gas and for oxidation of the process gas stream may be

specified. The module iteratively guesses the amount of fuel gas (and air) required to achieve the desired outlet conditions. The air required for the specified combustion of both the fuel and process gases is determined in the same way as done for the combustion air adder. The combustion products at the specified outlet temperature form the equipment outlet stream.

Incinerator Simulation

Simulation of the incinerator involves combining the equipment process feed stream with a specified air and fuel gas stream. The resulting combustion composition and temperature are found by an iterative adiabatic temperature calculation.

9. Effluent Stack

The stack inlet stream and outlet conditions determine the amount and concentration of pollutant resulting from the sulphur plant. Since pollution is under government regulation, the calculations used by this module have been patterned after those used by the Alberta Provincial Government Department of Health. Thus, the validity of the calculations is not assured, but agreement with the results of this government agency is.

The calculations which have been used assume reasonably level surrounding terrain and become invalid if the area

around the plant is mountainous or very hilly. The maximum pollutant gas concentration at ground level and the distance from the stack at which this maximum occurs are predicted using the Sutton equation with the Lowery modification(45).

Stack Simulation

The specification of stack height and top stack diameter are required for simulation. For both simulation and design, the ambient air temperature and stack exit temperature may be specified; otherwise they are assumed. Stack simulation results in the maximum sulphur dioxide ground concentration and the distance to the maximum being predicted for moderately stable and moderately unstable atmospheric conditions. Simulation corresponds exactly to the government calculations.

Stack Design

A straightforward method of determining the required stack height for a given stack inlet, stack velocity and specified maximum ground concentration was derived. For each of several specified exit stack velocities, the module finds the required stack diameter (top) and predicts the minimum stack height necessary.

The equations used for stack simulation and design, assuming ideal gas behaviour, are presented in Appendix A.9.

V. PROGRAM INPUT AND OUTPUT

A. Data Input

A module has been developed for program data input. This module inputs all the data necessary for the executive and the equipment modules that have been included. If more equipment modules are developed and additional data is required, the input module will have to be expanded to accommodate the additional input.

The two primary objectives of the method used for data input are:

1. a minimum amount of data should be required and from the program user's standpoint, the data input should be as simple as possible,
2. error checks should be used extensively to detect input data errors, and messages should accompany these checks to assist data correction.

Although it is impractical to check for all possible data errors and inconsistencies, an attempt has been made to detect most obvious errors. If errors are encountered during data input, the appropriate error messages are written and upon input completion, the job is aborted. This avoids the wasting of expensive computer time because of invalid input data.

The specified data should be chosen carefully, especially when the data in question may be optionally

given. The mode (simulation or design) in which a module operates depends upon the presence or absence of certain data. Some data that is essential for a module's calculations will be assumed if it is absent, but this is not true for all data. (See Appendix B.) Checking of data during input is primarily on that given; few checks are made to see that all necessary data is given. The only way to assure that the desired calculations are done is to give the correct, necessary data; if this is not done the results produced may be erroneous.

In order to achieve simplification of data input, a free format input (FFINP) method has been implemented. The main advantage of this technique is that the rigid format requirements of Fortran input are eliminated. Thus there is no need for data coding sheets etc. Also, data checking and optional data input are more easily handled using the FFINP approach. Job termination during data input and ambiguous error messages which frequently result from Fortran input errors are prevented. This should allow for all errors in a data set to be detected and corrected with a single run.

Free format input is achieved by reading a whole data card at once as an alphameric vector. The alphameric vector is then analyzed one character at a time to decode the integer, real and alphameric input data. The input of a given amount of data may be done using as many cards as is convenient and may be in any format the user desires.

The characters recognized by the FFINP routine are

CHARACTER		DESCRIPTION
	blank	- space separating data (delimiter)
0-9	numerals	- used to define integer or real data
E	exponent	- preceeds exponent (decimal shift) - implies a real value for the number
+, -	sign	- may be used with integer or real or real number's integer exponent
,	comma	- optional delimiter separating data
.	decimal	- implies a real value for the number
*	asterisk	- control character used to enclose data control messages
**	double asterisk	- control character used to force return to data analysis - signifies end of data segment
'	quote	- alphameric data control character - used to enclose alphameric data
C	comment	- denotes a data comment - the remainder of the card is ignored
<p>Note: - no imbedded blanks are allowed within a real or integer field (a blank is a data delimiter), - integers must not include decimals or exponents, - only ordering within a group is important, (ie. integers ordered w.r.t. integers etc.)</p>		

TABLE II. CHARACTERS RECOGNIZED BY FFINP ROUTINE

listed and described in Table II. It has been found that this method of input is far more versatile than the standard Fortran input. The FFINP routine has been generalized to achieve versatility; many equivalent ways of presenting a given data set are acceptable. An example illustrating several means of input of a given data set may be found in Appendix B.

The data required by the modules developed has been divided into five independent sections. The input of these sections need not be in a specific order and all sections are not necessarily used. Data input is data controlled rather than program controlled. Each data section is preceded by a control message to indicate the type of data following. This enables the input executive to call the appropriate input routine. Control is usually returned to the input routine several times within the section by the use of the ** data control characters. A control message indicating the end of the data section, or the end of all data, follows the section. An example of data using control messages and indicating the ends of sections and all data is included in Appendix B. The control messages which are recognized by the input program are as follows:

PROGRAM CONTROL PARAMETERS

MOLECULAR AND THERMODYNAMIC DATA

EQUIPMENT PARAMETER SPECIFICATIONS

EQUIPMENT PARAMETER ESTIMATES

STREAM SPECIFICATIONS

STREAM ESTIMATES

FLOWSHEET DATA

END

END OF ALL DATA

Note: - spelling is important but spacing of messages is not (eg. * e n d ofall data*),
 - control messages must be enclosed in asterisks and must be on a single card.

The data anticipated by each section and the manner in which this data is analyzed and stored will now be described.

1. Program Control Parameters

This section may be used to specify program options as distinct from calculational options. If this section is skipped, values for all the parameters are assumed. The data for this section is as follows:

- a. IDBUG(15) (integer,optional) - an output control vector.
 Its use is explained in the Program Output section. The first n elements may be specified where n is between 1 and 15. Each element must be in the range 0 - 5 and if not specified, elements are assumed to be zero.
- b. CRIT (real,optional) - a calculation convergence criterion. The smaller it is, the more rigorous iterative calculations become. All convergence

criteria used to check relative errors are scaled to this value. CRIT must be in the range 0 - 1 and if not specified, a value of 1.E-4 is assumed.

- c. 'NO OPTIMIZATION' (alphameric,optional) - if this input message is specified, the normal calculation sequence optimization is not done. Instead, a calculation sequence identical to the order in which the equipment is listed in *EQUIPMENT PARAMETER SPECIFICATIONS* is used.
- d. 'PRINT SUPPRESS' (alphameric,optional) - this input message results in a suppression of all output during the first pass of recycle loops. The option does not suppress output on succeeding passes and has no effect on output for calculations external to recycle loops.
- e. *END*

2. Molecular and Thermodynamic Data

This data section defines the atom types and molecular species present in the process reaction systems. Atomic symbols, weights and volumes are read and used for determination of molecular weights and volumes. Optional viscosity coefficients and the thermodynamic data required for stream composition calculations are read for each molecular specie included.

The atomic definition of the system is:

- a. ISYMB(5) (alphabetic,mandatory) - one to five single letter designations for atom types (eg. 'H' 'S'). All atom types present in the reaction system must be given - 5 maximum.
- b. ATMWT (real,mandatory) - the atomic weight of one of the above atoms.
- c. VATOM (real,mandatory) - the atomic volume of one of the above atoms. A reference for atomic volumes is Kern(46).

Note: - b. & c. are repeated for each of the atom types listed.

d. **

The molecular specie data is given as follows:

- e. NAME(4) (alphameric,mandatory) - chemical formula of molecular specie, using atom symbols defined. Must be 4 characters long and may use blanks, atom symbols and numerals 1 to 9. (eg. 'H2S ' 'S8 ').
- f. PHASE (alphabetic) - designates the phase of the above molecular specie. For gaseous species 'G' is optional, but for liquids, 'L' must be specified.
- g. V(2) (real,optional) - two coefficients for molecular viscosity. If specified, they must be for the functional form:

$$\text{viscosity} = V(1) + V(2)*T$$

where viscosity is in centipoises and

temperature is in degrees Fahrenheit.

If not specified, V(1) is assumed as 0.015 and

V(2) as 0.00002 .

h. A(14) (real,mandatory) - fourteen thermodynamic function coefficients. The first seven are used for the temperature range 300 to 1000 degrees Kelvin and the last seven for the range 1000 to 6000 degrees Kelvin. The coefficients must correspond to the NASA(30) functional format for the following thermodynamic properties:

heat capacity,

$$\begin{aligned} C_p/R = & A(1) + A(2).T + A(3).T^2 + A(4).T^3 \\ & + A(5).T^4 \end{aligned}$$

enthalpy,

$$\begin{aligned} H/RT = & A(1) + A(2).T/2 + A(3).T^2/3 + A(4).T^3/4 \\ & + A(5).T^4/5 + A(6)/T \end{aligned}$$

free energy,

$$\begin{aligned} F/RT = & A(1).(1-\ln T) - A(2).T/2 - A(3).T^2/6 \\ & - A(4).T^3/12 - A(5).T^4/20 + A(6)/T - A(7) \end{aligned}$$

i. **

Note: - e.,f.,g.,h. and i. are repeated for each molecular specie.

j. *END*

A maximum of 20 molecular species may be included.

A maximum of 5 elemental sulphur species may be given and only one water specie (vapor) is allowed.

3. Equipment Parameter Specifications

This data section is for the specification of equipment parameters such as tube diameter, length, cross-sectional area, outlet temperature, maximum flow rate and pressure drop etc. A different number of parameters are associated with each type of equipment. Inefficient storage utilization would result because of this variation, if the parameters for each equipment unit were stored in a single row of an equipment parameter matrix. Accordingly, all equipment parameters are stored in a single long vector. The initialization of this data section involves zeroing this vector and then allocating sections of the vector to the various equipment numbers. The length of the section devoted to an equipment number depends upon the corresponding equipment type. The location of an equipment's parameters in the vector is stored in an index.

The sequential parameters have an unique meaning for each type of equipment. The parameters for the types of equipment included, and their meaning are documented in Appendix B. Only those parameters that are specified need be given. Specified parameters, although read as positive real values, are stored negatively to indicate specification. This is to distinguish specified values from estimated or calculated values. The input of equipment parameter specifications is as follows:

First the equipment numbers and corresponding types are

defined. If 'NO OPTIMIZATION' is specified, the order of equipment numbers given here will be used for the calculation sequence.

The initialization of this section is as follows:

- a. INUMB (integer,mandatory) - the number by which a particular equipment unit is identified. The equipment number must be in the range 1 - 25.
- b. ITYPE (integer,mandatory) - the type of the equipment designated by the above equipment number. (eg. 1 = waste heat boiler, 9 = stack, etc.)

Note: - a. and b. are repeated for each equipment unit in the process flowsheet.

c. **

The equipment parameters are specified as follows:

- d. IEQIP (integer,mandatory) - a previously defined equipment number.
- e. IPAR (integer,mandatory) - the parameter number of the equipment parameter (of IEQIP) being specified.
- f. VALUE (real,mandatory) - the value of the equipment parameter being specified. VALUE is always positive.

Note: - e. and f. are repeated for each parameter of equipment number IEQIP being specified.

g. **

Note: - d.,e.,f., and g. are repeated for each equipment number for which some parameters are to be specified.

h. *END*

Equipment Parameter Estimates

The input of parameter estimates is identical to the last part of parameter specifications. The definition of equipment numbers and types is not required again. Parameter estimates must always come sometime after parameter specifications because the storage initialization is done during the specification. Parameter estimates are stored positively to distinguish them from specifications.

Equipment parameter estimates are given by following steps d., e., f. and g. repeatedly for each equipment number for which there are estimates. The estimates may be omitted, but if they are given, must follow a *EQUIPMENT PARAMETER ESTIMATES* control message.

4. Stream Specifications and Estimates

This section inputs specification of stream compositions and/or stream temperatures and pressures. For the complete design of a sulphur plant, only the feed acid gas stream and the fuel gas (sample composition) to the incinerator need to be specified. For simulation, air streams generally should be specified. If only segments of the plant are being done, or individual equipment units, additional stream specifications will be required.

Stream specifications are given as positive values but

are stored negatively as for equipment parameter specifications. Equipment inlet or outlet temperatures may be specified as stream parameters rather than the corresponding equipment parameters if this is convenient. If two or more possible means of specifying a variable exist, both are checked by the module. Stream estimates are stored as positive values and are indistinguishable from calculated stream values. Stream estimation is really only required if the stream in question may have to be assumed for recycle calculations.

The format for both stream specifications and stream estimates is:

- a. ISTRM (integer,mandatory) - the stream number for which the parameters are being specified. The stream number must be in the range 1 - 50.
- b. IPAR (integer,optional) - the number of the parameter of stream ISTRM being specified. The first 20 parameters may be used for stream mole numbers (moles/hr.) The 21st always refers to the stream temperature (deg. F.) and the 22nd to stream pressure (psia.) The order of the mole numbers corresponds to the order in which molecular species are listed under *MOLECULAR AND THERMODYNAMIC DATA*
- c. VALUE (real,mandatory) - the value of the appropriate mole number, temperature or pressure which is being specified or estimated. VALUE is always

positive.

Note: - b. and c. are repeated for each parameter being specified for stream ISTRM.

d. **

Note: - a., b., c., and d. are repeated for each stream for which some parameters are being specified or estimated.

e. *END*

If IPAR's are not used for the parameters of a stream being specified, it is assumed that all mole numbers are being specified. The last parameter is assumed to be pressure (22), the second last temperature (21) and the remaining twenty or fewer parameters are assumed to be the mole numbers. If the option of omitting IPAR's is used for more than one stream, a consistent number of parameters must be given.

5. Flowsheet Data

This data section is the encoded representation of the process flowsheet. The data is used to optimize the order of process calculations. During the calculations themselves, the flowsheet data is used to find the streams to and from the equipment unit of interest. The flowsheet data is presented as follows:

a. ISTRM (integer, mandatory) - a number used to identify the stream. The stream number must be in the range

1 - 50.

- b. IFROM (integer,mandatory) - the number of the equipment from which the stream originates. IFROM must be in the range 0 - 25. Zero indicates a plant feed (ignored during optimization).
- c. ITO (integer,mandatory) - the number of the equipment to which the stream is destined. ITO must be in the range 0 - 25. Zero indicates a plant product or discharge stream (ignored during optimization).
- d. IUNKN (integer,optional) - the number of stream unknowns associated with the stream. IUNKN is used exclusively during optimization and may be any positive number. If unspecified, IUNKN is assumed to be one.
- e. IFLAG (integer,optional) - a flag to indicate the type of the stream:

-1 = information stream,

0 = process stream,

1 = service stream.

If IFLAG is to be specified, IUNKN must also be specified. (ie. IFLAG must be the fifth integer.)

If not specified, IFLAG is assumed to be zero.

f. **

Note: - a.,b.,c.,d.,e., and f., are repeated for each stream in the flowsheet.

g. *END*

Note: - at the end of the last data section, irrespective

of the section that is last, a control message *END OF ALL DATA* must exist.

Examples of data for each of the described data sections may be found in Appendix B. Both logical examples (using the variable symbols defined in the previous sections) and numerical examples are included.

B. Program Output

The program output is completely governed by the output control vector, IDBUG, and the 'PRINT SUPPRESS' option. By appropriate definition of IDBUG, the output of results can be varied from essentially nothing to several hundred pages. The program has been divided into sections and each element of IDBUG pertains to a particular section. The sections are as follows:

1. waste-heat boiler,
2. in-line burner,
3. converter,
4. condenser,
5. adiabatic stream combiner,
6. stream combiner/divider,
7. combustion air adder,
8. incinerator,
9. stack

Note the correspondence to equipment types.

10. future,

11. future,
12. equilibrium compositions,
13. calculation optimization,
14. data input echo check,
15. executive functions.

For the first thirteen elements, the results of defining the element between 0 and 5 are as follows:

- 0 - no output,
- 1 - thesis format output of primary results,
- 2 - low level debug output plus above,
- 3 - moderate level debug output plus above,
- 4 - high level debug output plus above,
- 5 - complete debug output.

A detailed list of the output resulting from these options will not be given here.

If the option 'PRINT SUPPRESS' is used, the first 9 elements are effectively defined to be zero for the first calculation pass of recycle loops.

The fourteenth element is used to control whether a data echo check results. This echo check consists of a formatted output of input data, assumed data and derived data. The results of defining this IDBUG element are:

- 0 - no echo check,
- 1 - partial echo check,
- 2 - complete echo check.

The value of the element has absolutely no bearing on the output of data error messages for errors detected.

The fifteenth element pertains to executive functions. The defining of this element results in the following:

- 0 - no output,
- 1 - thesis format summary of calculations when process calculations have been completed.
- 2-5 - above plus recycle and other executive debug.

In particular, if a high debug output is imposed on the equilibrium calculations, a large amount of output will result. The debug on this section can be made quite extensive and since the calculations are iterative and are used frequently, more output than desired may result. The output resulting from the thesis format level may be seen in the appended examples.

VI. RESULTS AND DISCUSSION

A. Industrial Data

It was stated previously that one objective of this project was to compare extensively the program's numerical results with actual industrial data. Unfortunately, this objective has not been fully achieved. A virtually unlimited number of arbitrary plants may be designed and/or simulated with the program and many cases have been tried. However, the correspondence between the calculated results and actual plant conditions is necessary to establish how realistic the results are. For such a comparison, reasonably good quality plant data is essential.

Originally it was intended that a substantial amount of industrial data would be obtained at the outset of the project, and that this data would provide a guide for the program development. The data was not forthcoming, and so the development began without it. Only towards the completion of the project was any data obtained. At this stage, major modifications could not be easily made. Some changes were made and will be discussed shortly.

The industrial data acquired was neither as accurate nor as detailed as desired. "Research quality" data was not expected, but at least a small amount of high quality "industrial" data was anticipated. Some data was found to be useless for comparison purposes, and unfortunately some

of the best data "obtained", although closely matched, cannot be published since it is proprietary. The remaining data was not used because it was adequate, but only because it was all that was available.

Some specific shortcomings of the plant data recieved included:

- absence of important stream flows such as the plant air feed,
- insufficient and inaccurate temperature and pressure measurements throughout the plant,
- obvious data discrepancies,
- questionably valid stream compositions, and
- variation in the times at which samples and measurements were taken, particularly when the plant was not at the same steady conditions during the entire sampling period.

These shortcomings are not a reflection on the operating companies, who obviously take as much data as required to successfully operate their plants. Rather they are related to the data's usefulness for the desired comparison. For adequately testing the program and verifying its predictions, very accurate and detailed data is desireable. This quality of data may not be economically justifiable from an industrial standpoint.

It should be noted that obtaining compositions for sulphur plant streams is very difficult. The practical problems necessitate quenching of the sample streams and

removing water and liquid sulphur before analysis is done by chromatograph. Thus the water and sulphur contents of the streams are unknown. These difficulties however do not eliminate the critical need for exact stream compositions if an adequate comparison of calculated and actual plant data is to be done.

The scarcity of operating data can be at least partly justified by the foregoing. However, the fact that very little physical equipment specification data was accessible is less understandable. The latter data is essential if plant simulation (versus design) is to be done. For plant simulation, the feed streams and equipment specifications are used as input. The calculated inter-equipment compositions, temperatures and pressures can then be compared to those actually observed. In the design case, since temperatures and pressures must be specified, only compositions can be checked in the absence of equipment specifications.

In summary, while the data obtained from industry is sufficient for their purposes, it was neither accurate nor complete enough to adequately test the program's predictions.

B. Introduction of the Black Box Module

When some data was obtained, the observed operating temperatures and pressures were used as specifications for

designing corresponding sulphur plants. A problem in accommodating the given flowsheets was encountered: bridging those pieces of equipment for which no equipment module had been developed (e.g. gas-to-gas exchangers, direct fired heaters, etc.). This problem necessitated completing the whole plant design in sections beginning and ending at such equipment types. The difficulty was resolved by introducing a "black box" module.

Originally, if a stream S flowed from equipment node A to B, (and it was not necessary to assume stream S to begin the calculations), the executive would ensure that node A was calculated before node B. The calculations at node A would define stream S and there was no means of altering stream S before calculations at node B were done. By introducing a black box equipment module, an additional node between nodes A and B could be introduced to alter stream S before calculations at node B were done. The black box module then was really a dummy module to alter the stream temperature, pressure and/or composition.

The single equipment parameter associated with the black box is an equilibrium cutoff temperature. If not given, it is assumed negative (sulphur shift only). The outlet stream temperature and pressure are specified as

STREAM SPECIFICATIONS - if not specified, they are assumed the same as the inlet temperature and pressure (i.e. the black box has no effect). By means of this technique, all the flowsheets encountered were completed with single

runs of the program.

It should be noted that the black box may be used to replace a module such as the waste-heat boiler if the design of the boiler is not required. This results in a substantial saving of computer time, particularly if the boiler is in a process design recycle loop as it usually is.

C. Predictions of CS₂ and COS

It was found that the program consistently predicted less COS and (particularly) CS₂ throughout the plants designed than that observed industrially. It was felt the qualitative consistency precluded analysis errors and so an explanation was sought.

Most sulphur plants have some hydrocarbon in the feed and usually it is not exclusively methane. However, methane is the only hydrocarbon for which NASA format thermodynamic data is available. (This is a data limitation rather than a program limitation.) Because of the limitation, higher hydrocarbons were substituted with methane equivalent on either a carbon or an enthalpy basis. This introduced differences between specified and actual plant feeds, but it was expected the effects would be limited to the adiabatic flame temperatures.

It is quite conceivable, although not assured, that higher hydrocarbons contribute significantly to the formation of COS and CS₂. If this were the case, the

differences between calculated and actual COS and CS₂ stream concentrations would be partly explained. However, even in plants with methane the sole hydrocarbon in the feed, substantial amounts of CS₂ and COS were reported. The program invariably predicted significantly smaller amounts of COS and negligible amounts of CS₂.

The plant data showed that COS and CS₂ among other species are produced in the boiler and in most cases remain throughout the rest of the plant. Presumably then, their formation is related to the flame reaction in the boiler. The calculations done by the program involve complete thermodynamic equilibrium at a theoretical bulk gas adiabatic flame temperature. Equilibrium predictions of COS and CS₂ increase with temperature at the flame temperatures and although it is impossible to obtain more than the equilibrium amount at this temperature, it is possible at different conditions. It is quite plausible that in the complicated and drastic temperature and concentration gradients involved in the flame reaction, CS₂ and COS are produced in high temperature zones and due to kinetic limitations, do not disappear before being quenched in a cooler temperature zone. A kinetic flame analysis, impossible at this time, would be necessary to prove or disprove this hypothesis. Assuming both plant analyses and the thermodynamic data are correct, this explanation of the discrepancies seems the most plausible at this time.

D. Introduction of a Secondary Cutoff Temperature

The flame reaction in the boiler accounts for production of more than COS and CS₂. At the high temperatures involved and increasing with temperature, significant amounts of CO and H₂ are produced along with negligible amounts of several other species. As the flame products are cooled in the boiler, reaction quenching takes place. This has been accounted for by the introduction of the boiler equilibrium cutoff temperature previously described in Chapter III. This cutoff temperature pertains to all species. It was felt that equilibrium was achieved in the converters and that a single cutoff temperature for the boiler would suffice. This does not appear to be the case.

Plant data shows that H₂ and CO produced in the boiler persist through the converters to the plant tail gas. Theoretical equilibrium in the first converter predicts that nearly all of these species should disappear to form H₂O and CO₂. It would appear that the converters principally catalyze the primary reaction involving H₂S and SO₂. Equilibrium for this reaction does not seem to be completely achieved industrially and equilibrium conversions involving other reactions often are not even approached. For given feed conditions, the theoretical converter equilibrium calculations result in too high adiabatic reaction temperatures and a better than actual H₂S/SO₂ ratio. The

latter results from the fact that the presence of H_2 and CO is accompanied by the formation of more SO_2 than if they are absent. This ratio becomes quite critical towards the end of the plant - if the ratio differs from two, a reactant deficiency occurs before complete conversion is attained. Thus calculated converter recoveries and overall plant recoveries tend to be slightly higher than those industrially observed.

A simple method of preventing conversion of components which are not actually converted was devised. The method involves "masking" the species in question during the equilibrium calculations. A secondary cutoff temperature is associated with this masking. Just before the equilibrium calculations begin, a masking routine is called (subroutine FAKER). If compositions for either a boiler or a converter are being calculated, and if the temperature is below the specified secondary cutoff, the number of gaseous molecular species is temporarily reduced (for the duration of the free energy minimization) by the number of species to be masked. By masking the last four species (CO_2 , CS_2 , CO and H_2) much closer agreement with industrial data was possible. (The number of gaseous species not to be masked and the secondary cutoff temperature were input from a remote terminal rather than with the rest of the input data on cards.)

Even with masking, the conversions in the first converter appear to be consistently high, judging by the converter outlet temperatures. Although the calculations

involved are done adiabatically, there are actually heat losses involved. This would seem to be confirmed by reported converter bed temperatures being higher than the outlet stream temperature. The calculations result in a larger portion of the conversion being done in the first converter, too low a second converter conversion and a higher overall plant conversion.

A further application of the masking is in direct oxidation plants and 2/3 bypass Claus plants, where it is found that the hydrocarbons included in the converter feeds are not combusted as equilibrium predicts. Thus, for plants with hydrocarbons in the converter inlets, the hydrocarbons should probably be included in those molecular species that are masked.

E. Examples of Program Use

Five of the many plants designed (or simulated) have been included in Appendix E. A plant description, flowsheet, the program input data (card image) and the resulting output for each example are included. All of the examples are for straight through Claus type plants - however other types of plants can and have been tried successfully. Although the examples included are for complete plants, it is by no means necessary to do a complete plant. One or several independent pieces of equipment or segments of a plant can also be easily handled.

A brief description of the examples and a summary of some of the results will be given here. For more detailed documentation, the reader is referred to Appendix E.

Example 1. This example is a general design of a complete sulphur plant, utilizing both boiler bypass and inline burner reheating. Two converters and three condensers are used. A boiler cutoff temperature of 1600 Deg. F. was specified, but masking was not used for this example. The output illustrates the format of low level design output (with the print suppress option used) and of the calculation summary. The acid gas feed is an industrial feed, but this is the only data for the plant, so no comparison with industrial data can be made.

Example 2. This example is another general plant design. In this case, no summary was desired and the print suppress option was not used. Note that results for both passes through the recycle loop are included. In this plant reheat was by boiler bypass and a gas-to-gas exchanger. The latter was simulated using two black boxes. The feed and operating conditions were industrially specified. However, the only data available for comparison was three (calculated) plant temperatures. A temperature comparison is shown in Table III.

The analysis for this example includes a smaller set of molecular species (possibly introducing errors) than was

TEMPERATURE LOCATION	TEMPERATURE PREVIOUSLY CALCULATED (INCLUDED AS PART OF THE DATA)	TEMPERATURE CALCULATED IN THIS WORK BY THE PROGRAM (1)
	(DEG. F.)	(DEG. F.)
Boiler Adiabatic Flame	(2) 2285	2415
No. 1 Converter Exit	582	584
No. 2 Converter Exit	445	438

- (1) These temperatures were matched as closely as possible by varying the primary (boiler) cutoff temperature to control the conversion achieved in the boiler (temperature used was 1800 Deg. F.)
- (2) This temperature is the given calculated reaction chamber outlet temperature which is supposedly about 100 Deg. F. lower than the calculated adiabatic flame temperature.

TABLE III. PLANT TEMPERATURE COMPARISON FOR EXAMPLE 2.

normally used. This was done for compatibility with the calculations done by the data source.

Example 3. This example has been included to illustrate the simulation capability of the program. As stated earlier, almost no equipment (simulation) specifications were obtained and therefore total plant simulation could not be done. The simulation done for this example utilized the results of a previous program design for the plant, except for the condenser specifications which were given. Both the boiler cutoff temperature and the masking temperature were set to 1850. Deg. F. COS, CS₂, CO and H₂ were masked.

The data for the plant included the measured acid gas and combustion air flows and compositions. In the data it was reported that "there was serious doubt about the reliability of the air flows". Chromatographic analyses (on a dry basis) were taken of several important streams over a period of time. The remaining stream compositions and the water and sulphur content of all streams were then calculated by material balances. The boiler bypass flowrates were calculated using a heat balance. Since there appeared to be a discrepancy in the results of these calculations, the program was used to find the amounts of boiler bypass required to achieve the observed combined temperatures (done during the design phase).

A comparison of the given (calculated) compositions for several streams to that calculated by the program with

STREAM COMPOSITIONS - MOLE PERCENT ON A SULPHUR FREE BASIS *

NO. 1 CONDENSER EXIT STREAM				NO. 2 CONDENSER EXIT STREAM			
	DATA SOURCE	PROGRAM PREDICTION		DATA SOURCE	PROGRAM PREDICTION		
		MASKING	NO MASKING		MASKING	NO MASKING	
A	0.67	-	-	0.65	-	-	
N2	54.83	55.88	55.88	55.83	57.18	57.30	
CO	0.69	0.52	0.52	0.61	0.53	TR	
CO2	5.20	5.54	5.54	5.78	5.67	6.28	
COS	0.34	0.07	0.07	0.02	0.06	TR	
H2S	5.03	6.58	6.56	1.80	2.06	3.74	
CS2	0.03	TR	TR	0.01	TR	0.0	
S02	2.89	3.37	3.36	0.93	1.11	0.90	
H2	2.57	1.47	1.47	2.57	1.50	TR	
H2O	27.74	26.59	26.60	31.79	31.88	31.78	
	-----	-----	-----	-----	-----	-----	
TOTAL	99.99	100.02	100.00	100.00	99.99	100.00	

* The boiler bypasses used were 537 moles/hr. and 505 moles/hr. rather than the reported values of 934 and 968 moles/hr.

STREAM COMPOSITIONS - MOLES PER HOUR ON A SULPHUR FREE BASIS

	NO. 3 CONDENSER EXIT STREAM			NO. 4 CONDENSER EXIT STREAM		
	DATA SOURCE	PROGRAM MASKING	PREDICTION NO MASKING	DATA SOURCE	PROGRAM MASKING	PREDICTION NO MASKING
A	34.0	-	-	34.7	-	-
N2	2847.5	2864.9	2864.9	2849.6	2864.9	2864.9
CO	29.5	26.5	TR	29.5	26.5	0.0
CO2	284.3	284.1	314.2	284.3	284.1	314.2
COS	0.7	3.5	TR	0.7	3.5	TR
H2S	47.2	47.5	112.8	27.6	15.0	97.6
CS2	0.3	TR	0.0	0.3	TR	0.0
S02	31.8	27.7	7.8	18.2	11.5	0.2
H2	80.7	75.1	TR	72.0	75.1	TR
H2O	1649.0	1653.0	1662.7	1677.4	1685.4	1678.0
	-----	-----	-----	-----	-----	-----
TOTAL	5005	4982	4966	4994	4966	4955

TABLE IV. COMPARISON OF PLANT STREAMS FOR EXAMPLE 3.

masking (as in Appendix E., Example 3.), and without masking is presented in Table IV.

The type of condensers in this plant were not the type for which the condenser module was written. However, since so little equipment specification data was obtained, this data was used. The condensers are horizontal and besides producing steam, a large amount of water is recirculated and heated, whereas the condenser module was developed for vertical condensers solely producing steam. Only the design pressure was available for these condensers and whether they are operated at design pressure (exactly) is not known. This is of considerable importance in the simulation, since the steam pressure defines the shell side steam temperature and so has a large effect on the heat transferred. Finally, the last condenser is really an economizer and doesn't produce steam at all. It was simulated as a vertical steam producing condenser in spite of this.

A comparison of the condensers, converters and overall plant performance for this example may be found in Table V.

Example 4. This example illustrates the design of a plant with no output but the calculation summary. Masking was used with both the primary (boiler) and secondary (masking) cutoff temperatures set to 2000. Deg. F. No recycling of calculations was required in this case since all inline burner feeds as well as the main boiler feed were specified. The inline burner feeds include fuel gas as well as the

CONDENSER	INLET TEMPERATURE (DEG. F.)			OUTLET TEMPERATURE (DEG. F.)		
	ORIGINAL PLANT DESIGN	MEASURED	PROGRAM CALCULATED /SPECIFIED	ORIGINAL PLANT DESIGN	MEASURED	PROGRAM CALCULATED
1.	550	552	552	350	296 *	346
2.	568	597	608	335	303	342
3.	426	383	383	335	298 *	321
4.	415	413	407	265	288	269

CONVERTER	PERCENT CONVERSION OF INLET SULPHUR **			INLET TEMPERATURE (DEG. F.)	OUTLET TEMPERATURE (DEG. F.)	
	DATA SOURCE	PROGRAM PREDICTION			DATA SOURCE	PROGRAM PREDICTION
1.	68.2	68.4		490	597	608
2.	62.5	59.4		470	517	511
3.	41.6	61.8		388	413	407

* Note that these temperatures are below the saturation temperature of the shell side steam at the specified design pressure.

** The plant recovery predicted by the program was 97.2 percent versus a reported 96.4 percent recovery and 97.1 percent inlet sulphur conversion.

TABLE V. COMPARISON OF CONDENSERS AND CONVERTERS FOR EXAMPLE 3.

STREAM COMPOSITIONS - MOLES PER HOUR ON A SULPHUR FREE BASIS

SPECIE	BOILER EXIT		NO. 1 CONVERTER EXIT		NO. 2 CONVERTER EXIT		NO. 3 CONVERTER EXIT	
	DATA	PROGRAM	DATA	PROGRAM	DATA	PROGRAM	DATA	PROGRAM
H2	210.8	220.2	273.8	220.2	250.9	232.1	212.8	248.6
A	62.6	.	62.0	.	64.9	.	67.2	.
N2	5227.7	5270.0	5179.7	5270.0	5420.6	5439.0	5617.3	5574.5
CO	89.7	205.4	90.9	205.4	84.2	218.2	96.0	235.0
CO2	1194.6	1143.6	1204.1	1143.6	1264.0	1167.8	1292.8	1188.9
COS	47.5	16.4	38.8	16.4	24.5	16.7	23.9	17.3
CS2	33.7	0.1	31.7	0.1	30.1	0.1	28.5	0.1
H2S	623.8	593.4	313.2	144.5	95.2	52.8	88.7	37.0
S02	305.8	296.8	145.3	72.4	40.8	28.5	33.1	12.4
H2O	2463.1	2486.0	2746.6	2934.9	3035.2	3099.2	3126.8	3183.5
	-----	-----	-----	-----	-----	-----	-----	-----
TOTALS	10,259	10,334	10,050	10,180	10,310	10,291	10,587	10,515

TABLE VI. PLANT STREAM COMPARISON FOR EXAMPLE 4.

CONVERTER	PERCENT CONVERSION OF INLET SULPHUR		INLET TEMPERATURE (DEG. F.)		OUTLET TEMPERATURE (DEG. F.)	
	DATA SOURCE	PROGRAM PREDICTION	DATA SOURCE	PROGRAM PREDICTION	DATA SOURCE	PROGRAM PREDICTION
1.	46.3	74.3	455 (445)	445	550	557
2.	62.8	60.7	425	427	498	454
3.	18.0	43.1	398	398	403	407
PERCENT OF INLET SULPHUR						
REACTION FURNACE CONVERSION			REPORTED BY DATA SOURCE	CALCULATED BY PROGRAM		
			66.3	70.8		
TOTAL PLANT RECOVERY			93.7	97.2		

TABLE VII. PLANT PERFORMANCE COMPARISON FOR EXAMPLE 4.

usual acid gas. There is uncertainty in the data as to the distribution of the combustion air between the burners and the boiler. A comparison of several compositions for this example is to be found in Table VI. Table VII contains a comparison of the converter performances.

Example 5. This example is another design case using masking. Only the condensers are "turned on" for the calculation print-out. A summary of all calculations is included. The data for this plant included the primary plant feed and inline burner feeds, one condenser's equipment specifications and several stream compositions. It is admitted that the reported compositions have too high a hydrogen content (proved by independent analyses). The single condenser which was specified (No. 2) was simulated.

Table VIII contains a comparison of the converters and condenser performances, while Table IX contains a comparison of several plant streams for this example.

The results of all the examples included, although interesting, are not conclusive. The data recieved was not exact enough for a definite comparison to be made. It has been found that very small changes in something like the air flow to the plant has a large effect on the overall plant performance, at least from a calculational standpoint. The comparisons done do show that reasonable plant design and simulation of sulphur plants can be done using the program.

CONVERTER	INLET TEMPERATURE (DEG. F.)		OUTLET TEMPERATURE (DEG. F.)		TEMPERATURE DIFFERENCE (DEG. F.)	
	DATA SOURCE	PROGRAM PREDICTION	DATA SOURCE	PROGRAM PREDICTION	DATA SOURCE	PROGRAM PREDICTION
1.	490	597	492	594	107	102
	399	422	389	406	23	17
CONDENSER						
2.	597	340	594	313	257	281

TABLE VIII. COMPARISON OF CONVERTERS AND CONDENSER FOR EXAMPLE 5.

STREAM COMPOSITIONS - MOLE PERCENT ON A DRY BASIS

MOLECULAR SPECIE	BOILER EXIT		NO. 1 CONVERTER EXIT		NO. 2 CONVERTER EXIT	
	DATA SOURCE	PROGRAM PREDICTION	DATA SOURCE	PROGRAM PREDICTION	DATA SOURCE	PROGRAM PREDICTION
CO2	11.34	11.51	13.28	12.05	12.98	12.21
H2S	4.40	7.10	2.28	1.67	1.33	0.20
SO2	1.79	4.46	1.12	2.55	0.69	1.99
COS	0.62	0.15	0.30	0.16	0.40	0.16
CS2	TR	TR	0.14	TR	0.09	TR
CO	0.70	1.98	0.70	2.18	0.68	2.24
H2	7.03	2.73	5.57	2.97	6.75	3.03
N2	74.12	72.05	76.61	78.44	77.00	80.16
O2	0.	0.	0.	0.	0.08	0.
	-----	-----	-----	-----	-----	-----
	100.00	99.98	100.00	100.02	100.00	99.99

TABLE IX. PLANT STREAM COMPARISON FOR EXAMPLE 5.

VII. CONCLUSIONS

1. A generalized executive program has been developed to supervise process calculations. This executive, together with the necessary equipment module subroutines, has been successfully applied to designing and simulating a number of sulphur recovery plants.
2. A method of optimizing the order of process calculations has been developed by extending a method presented in the literature. The optimization method has minimized (to the true optimum) the number of recycle assumptions necessary to complete the process calculations for all of the many flowsheets tried.
3. A program package has been developed for calculating thermodynamic equilibrium compositions involving complex reaction systems and large numbers of molecular species. A minimization of free energy technique presented in the literature has been adapted for use with the sulphur recovery reaction system. This method has been found to be efficient, versatile and very stable. The equilibrium approach seems to be reasonably suitable for the sulphur plant application if restrictions such as those described are imposed.
4. A comparison of the program results with industrial data has been attempted. Reasonable, but not exact agreement with the data has been achieved. Due to the uncertainty

of the data, however, few definite conclusions regarding the validity of the program's predictions can be made. The predictions of COS and CS2 appear to be lower than those measured, and usually calculated converter and overall plant recoveries are slightly higher than those actually obtained.

VIII RECOMMENDATIONS

1. It is felt that the design of process equipment should be divorced, in future, from the material and energy balance calculations, if the two are essentially independent. The executive type of program is best suited to pure material and energy balance calculations. A substantial waste of computing time results when the design is integrated if either the design is not required or the equipment in question is within a recycle loop. The boiler and condensers are good examples of this. Using the recommended approach, the equipment design that is required is done separately, using the results of the material and energy balance calculations. If the two types of calculations are inter-related, as for simulation, then they must be done together.
2. More effort should be devoted to closely predicting stream compositions. As a prerequisite for this, a conscientious attempt to obtain some high quality industrial data should be made. Additional thermodynamic data for hydrocarbons may also be beneficial. Once such data was obtained, the method of calculating compositions could be refined to reproduce actual compositions. In this regard, the introduction of a fractional approach to equilibrium might prove to be

advantageous. If such an equilibrium approach fails to adequately predict reality, it may be necessary to use a kinetic approach once sufficient kinetic data becomes available.

3. Additions to the program can be made to improve its versatility for the sulphur plant application. Two of the many possible additions are:
 - i. a module similar to the adiabatic stream combiner (or a modification of this module) which would recycle information to control the combiner outlet temperature. The information recycled in this case would regard a previous equipment outlet temperature rather than a previous stream split. Such a module could be used for instance in a 2/3 bypass plant to set the boiler outlet temperature so that when this stream was combined with the bypass, the desired first converter inlet temperature would result.
 - ii. a module, similar to the air adder module described, which would predict excess or deficient air requirements to the plant. The module would be used for maintaining a two to one ratio of H_2S to SO_2 in the plant tail gas. This would be especially useful when H_2 and CO are present throughout the plant and air requirements are accordingly affected.
4. Because of the generality of the executive program, it is not limited to the sulphur plant application. By appropriate addition of equipment modules, the program

can be applied to any process calculations. For instance, by including a distillation column module and perhaps additional modules, the gas plants normally associated with sulphur plants could also be designed or simulated. The scope of possible applications of the executive is virtually limitless.

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APPENDIX A

THIS APPENDIX CONTAINS A LIST OF THE PRIMARY EQUIPMENT
MODULE EQUATIONS. THE EQUATIONS HAVE BEEN DIVIDED INTO TEN
SECTIONS - EACH SECTION IS CONCLUDED WITH THE NOMENCLATURE
FOR THAT SECTION. WHERE FEASIBLE, THE NOMENCLATURE USED IS
CONSISTENT WITH THE PROGRAM - FORTRAN MATHEMATICAL NOTATION
IS USED EXCEPT FOR CONTINUATION OF ONE LINE TO THE NEXT.

THE APPENDIX SECTIONS ARE -

A.1.	WASTE HEAT BOILER.	A-2
A.2.	IN-LINE BURNER	A-5
A.3.	CONVERTER	A-6
A.4.	CONDENSER	A-8
A.5.	ADIABATIC STREAM COMBINER	A-13
A.6.	STREAM COMBINER/DIVIDER	A-14
A.7.	COMBUSTION AIR ADDER	A-15
A.8.	INCINERATOR	A-16
A.9.	STACK	A-17
A.10.	MISCELLANEOUS	A-19

A.1. WASTE HEAT BOILER

A.1.1 TUBE PASS TOTAL HEAT LOSS CALCULATION.

$$QTOT = QCONV + QRAD$$

-- CONVECTIVE HEAT LOSS (REF. VALDES(37))

$$QCONV = UCONV * AREA * DTLM$$

$$AREA = 3.14159 * TDIAM/12 * TLONG * TNUMB$$

$$DTLM = ((TFEED-TSHL1) - (TEMP-TSHL2)) / ALOG((TFEED-TSHL1) / (TEMP-TSHL2))$$

$$UCONV = 1 / (1/HG + RGF + RM + RS + 1/HS)$$

$$HG = 16.6 * (GT/3600)^{0.8} * CPAVG / TDIAM^{0.2}$$

$$GT = 144 * TMASS / (TNUMB * 3.14159 * TDIAM^2 / 4)$$

-- RADIATION HEAT LOSS (REF. HOTTEL(38))

$$QRAD = (EPSP + 1) / 2 * 0.1713E-8 * AREA * (EMIS * TMENR^4 - ABSOR * TWALR^4)$$

$$EMIS = FCN(PL) / TMENR$$

$$ABSOR = FCN(PL * TWALR/TMENR) / TMENR * (TMENR/TWALR)^{0.5}$$

$$PL = (PRESS/14.7) * BEAML * RPPRS$$

$$BEAML = TDIAM/12 * 0.9$$

$$RPPRS = SUM(YAVG(I) * RADCT(I)) / YTOT$$

A.1.2 TUBE PASS PRESSURE DROP (REF. VALDES(37))

$$DELPC = A1 * (FF/PHI + A2) * (GT/1.E5)^2$$

$$A1 = 5 * TLONG / (TDIAM * RHO)$$

$$A2 = 0.0416 * TDIAM / TLONG$$

$$FF = 0.079 / RE^{0.25}$$

$$RE = 0.0344 * TDIAM * GT / AVGMU$$

$$PHI = (AVGMU / WALMU) ** 0.14$$

$$RHO = TMASS * PRESS / (10.73 * YTOT * TMENR)$$

$$AVGMU = SUM(YM * VIS(TMEAN)) / SUM(YM)$$

(REF. PERRY(47))

$$WALMU = SUM(YM * VIS(TWALL)) / SUM(YM)$$

$$VIS(TEMPERATURE) = RMU(I) + SMU(I) * TEMPERATURE$$

$$YM(I) = YAVG(I) * WTMOL(I) ** 0.5$$

A.1.3 BOILER BYPASS STREAM CALCULATION

$$BYPASS \text{ NO. } 3 = BSTREAM * BYPASS \text{ RATIO NO. } 3$$

$$BYPASS \text{ NO. } 2 = (BSTREAM - BYPASS \text{ NO. } 3) \\ * BYPASS \text{ RATIO NO. } 2$$

$$BYPASS \text{ NO. } 1 = (BSTREAM - (BYPASSES \text{ NO. } 3 + \text{ NO. } 2)) \\ * BYPASS \text{ RATIO NO. } 1$$

NOMENCLATURE FOR SECTION A.1

ABSOR	-	GASEOUS ABSORPTIVITY AT TUBE WALL TEMPERATURE
AREA	-	TUBE PASS HEAT TRANSFER AREA (SQ.FT)
AVGMU	-	GAS VISCOSITY AT MEAN TUBE PASS TEMP. (CP)
A2	-	PRESSURE DROP END EFFECT TERM
BEAML	-	AVERAGE RADIATING BEAM LENGTH (FT)
BSTREAM	-	TOTAL BOILER STREAM EXIT SECOND LAST PASS
CPAVG	-	AVERAGE STREAM HEAT CAPACITY (BTU/LB.DEG.F)
DELPC	-	CALCULATED TUBE PASS PRESSURE DROP (PSI)
DTLM	-	LOG MEAN TEMPERATURE DIFFERENCE FOR PASS (DEG.F)
EMIS	-	GASEOUS EMISSIVITY AT MEAN PASS TEMPERATURE
EPSP	-	(= 0.8) TUBE WALL EMISSIVITY
FF	-	FANNING FRICTION FACTOR
GT	-	MASS VELOCITY THROUGH TUBE PASS (LB/SQ.FT.HR)
HG	-	TUBE SIDE CONVECTIVE HEAT TRANSFER COEFFICIENT FOR PASS (BTU/HR.SQ.FT.DEG.F)
HS	-	(= 2000.) STEAM SIDE HEAT TRANSFER COEFFICIENT
PL	-	PRODUCT OF BEAM LENGTH AND RADIATING GAS PARTIAL PRESSURE (USED TO GET EMIS AND ABSOR) (FT.ATM.)
PRESS	-	INLET TUBE PASS PRESSURE (PSIA)
QCONV	-	TUBE PASS HEAT LOSS FROM CONVECTION (BTU/HR)
QRAD	-	TUBE PASS HEAT LOSS FROM RADIATION (BTU/HR)
QTOT	-	TOTAL HEAT LOSS FROM ONE BOILER PASS (BTU/HR)

RADCT	- RADIATING COMPONENT FLAG VECTOR - VECTOR ELEMENTS ARE 1 FOR RADIATING COMPONENT, 0 FOR NONRADIATING
RE	- REYNOLD'S NUMBER
RGF	- (= 0.005) GAS SIDE FOULING RESISTANCE
RHO	- AVERAGED STREAM DENSITY (LB/CU.FT.)
RM	- (= 0.0001) TUBE WALL RESISTANCE TO HEAT TRANSFER
RMU	- VECTOR CONTAINING FIRST OF TWO VISCOSITY COEFFICIENTS FOR EACH MOLECULAR SPECIE
RPPRS	- RADIATING GAS PARTIAL PRESSURE (ATM.)
RS	- (= 0.0005) STEAM SIDE FOULING RESISTANCE
SMU	- VECTOR CONTAINING SECOND OF TWO VISCOSITY COEFFICIENTS FOR EACH MOLECULAR SPECIE
TDIAM	- PASS TUBE DIAMETER (INCHES)
TEMP	- PASS OUTLET TEMPERATURE (DEG.F) (KNOWN FOR DESIGN CASE, ITERATIVELY ESTIMATED FOR SIMULATION CASE).
TFEED	- PASS INLET TEMPERATURE (DEG.F)
TLONG	- PASS TUBE LENGTH (FT)
TMASS	- TOTAL TUBE PASS STREAM MASS (LB)
TMEAN	- AVERAGE STREAM TEMPERATURE (DEG.F)
TMENR	- MEAN TUBE PASS TEMPERATURE (DEG.R)
TNUMB	- NUMBER OF TUBES IN THE BOILER PASS
TSHL1	- STEAM TEMPERATURE AT PASS INLET (DEG.F)
TSHL2	- STEAM TEMPERATURE AT PASS OUTLET (DEG.F)
TWALL	- TUBE WALL TEMPERATURE (= SULPHUR DEW PT.) (DEG.F)
TWALR	- TUBE WALL TEMPERATURE (DEG.R)
UCONV	- OVERALL CONVECTIVE HEAT TRANSFER COEFFICIENT FOR TUBE PASS (BTU/HR.SQ.FT.DEG.F)
VIS	- SPECIE VISCOSITY (FUNCTION OF TEMPERATURE) (CP)
WALMU	- GAS VISCOSITY AT TUBE WALL TEMP. (CP)
WTMOL	- VECTOR OF SPECIE MOLECULAR WEIGHTS
YAVG	- VECTOR OF MOLE NUMBERS OF AVERAGE PASS STREAM
YTOT	- TOTAL MOLES IN AVERAGE PASS STREAM

A.2. IN-LINE BURNER

A.2.1 COMBUSTION CHAMBER SIMULATION

$$\text{HRELS} = \text{THRLS} / \text{VOLUM}$$

$$\text{RTIME} = \text{VOLUM} * 3600 * \text{PRESS} / 10.73 / (\text{TEMP} + 460) / \text{YTOT}$$

$$\text{VOLUM} = 3.14159 * (\text{DIAM}/12)^2 * \text{LNGTH} / 4$$

$$\text{THRLS} = \text{ENTHALPY}(\text{PRODUCTS AT FLAME TEMPERATURE}) - \text{ENTHALPY}(\text{PRODUCTS AT INLET TEMPERATURE})$$

A.2.2 COMBUSTION CHAMBER DESIGN

$$\text{VOLUM1} = \text{RTIME} * 10.73 * (\text{TEMP} + 460) * \text{YTOT} / 3600 / \text{PRESS}$$

$$\text{VOLUM2} = \text{THRLS} / \text{HRELS}$$

$$\text{VOLUM} = \text{MAX}(\text{VOLUM1}, \text{VOLUM2})$$

$$\text{LNGTH} = (\text{VOLUM} * 64 / 3.14159)^{(1/3)}$$

$$\text{DIAM} = 12 * (\text{VOLUM} * 4 / (3.14159 * \text{LNGTH}))^{0.5}$$

NOMENCLATURE FOR SECTION A.2

DIAM	-	REACTION CHAMBER DIAMETER (INCHES)
HRELS	-	UNIT VOLUME HEAT RELEASE (BTU/HR.CU.FT)
LNGTH	-	REACTION CHAMBER LENGTH (FT)
PRESS	-	REACTION CHAMBER PRESSURE (PSIA)
RTIME	-	REACTION CHAMBER RESIDENCE TIME (SEC)
TEMP	-	REACTION ADIABATIC FLAME TEMPERATURE (DEG.F)
THRLS	-	TOTAL REACTION HEAT RELEASE (BTU/HR.)
VOLUM	-	REACTION CHAMBER VOLUME (CU.FT)
VOLUM1	-	REACTION CHAMBER VOLUME REQUIRED FOR SPECIFIED FLAME REACTION RESIDENCE TIME (CU.FT)
VOLUM2	-	REACTION CHAMBER VOLUME REQUIRED FOR SPECIFIED MAXIMUM UNIT VOLUME HEAT RELEASE (CU.FT)

A.3. CONVERTER -----

A.3.1 CONVERTER BED SIMULATION

$$\text{VOLUM} = \text{XAREA} * \text{DEPTH}$$

$$\text{FLOWR} = \text{YTOT} / \text{VOLUM}$$

$$\text{VELMX} = \text{VGAS} / \text{XAREA} / 3600$$

$$\text{VGAS} = 10.73 * T * \text{YTOT} / P$$

$$P = \text{PRESS} - 0.2$$

$$T = \text{TFEED} + 25. + 460.$$

A.3.2 CONVERTER BED DESIGN

$$\text{VOLUM} = \text{YTOT} / \text{FLOWR}$$

$$\text{XAREA} = \text{VGAS} / \text{VELMX} / 3600$$

$$\text{DEPTH1} = \text{VOLUM} / \text{XAREA}$$

$$\text{DEPTH} = \text{MAX}(\text{DEPTH1}, 3.0)$$

A.3.3 CONVERTER BED PRESSURE DROP

$$\text{DELTP} = 8.32 * \text{DEPTH} * \text{GT}^2 / \text{PDIAM}$$

$$\text{GT} = \text{TMASS} / 3600 / \text{XAREA}$$

A.3.4 CONVERTER DEW POINT CHECKING

$$\text{TINCR} = (\text{TEMP} - \text{TFEED}) / 5$$

$$\text{PINCR} = \text{DELTP} / 5$$

$$\text{YINCR} = (\text{YCOMP} - \text{YFEED}) / 5$$

$$\text{TDIFF} = (\text{TEMP}' - \text{TDEW})$$

$$\text{TDEW} = \text{FCN}(\text{YCOMP}')$$

NOMENCLATURE FOR SECTION A.3

DELTP	-	PRESSURE DROP ACROSS CONVERTER BED (PSI)
DEPTH	-	CONVERTER BED DEPTH (FT)
DEPTH1	-	BED DEPTH REQ'D BY SPECIFIED MAX. MOLAL FLOWRATE
FLOWR	-	MOLAL FLOWRATE THRU BED (MOLES/HR.CU.FT.CATALYST)
GT	-	MASS VELOCITY THROUGH BED (LB/SQ.FT.SEC)
P	-	PRESSURE AT WHICH GAS VOLUME IS EVALUATED (PSIA)
PDIAM	-	AVERAGE CATALYST PARTICLE DIAMETER (INCHES)
PINCR	-	DEW CHECK INTERVAL PRESSURE LOSS (PSIA)
PRESS	-	CONVERTER INLET PRESSURE (PSIA)
T	-	TEMP. AT WHICH GAS VOL. IS EVALUATED (DEG.R)
TDEW	-	DEW CHECK INTERVAL OUTLET DEW POINT TEMP. (DEG.F)
TDIFF	-	DIFFERENCE BETWEEN BED AND DEW POINT TEMP.'S
TEMP	-	CONVERTER OUTLET TEMPERATURE (DEG.F) (DETERMINED BY ITERATIVE ADIABATIC CALCULATION)
TEMP'	-	DEW CHECK INTERVAL OUTLET TEMPERATURE (DEG.F)
TFEED	-	CONVERTER INLET TEMPERATURE (DEG.F)
TINCR	-	DEW POINT CHECK TEMPERATURE INTERVAL (DEG.F)
TMASS	-	TOTAL MASS OF STREAM PASSING THROUGH BED (LB/HR)
VELMX	-	SUPERFICIAL VELOCITY THROUGH BED (FT/SEC)
VGAS	-	VOLUME OF GAS PASSING THROUGH BED (CU.FT/HR)
VOLUM	-	CONVERTER BED VOLUME (CU.FT)
XAREA	-	CONVERTER BED CROSS-SECTIONAL AREA (SQ.FT)
YCOMP	-	CONVERTER OUTLET EQUILIBRIUM COMPOSITION
YCOMP'	-	DEW CHECK INTERVAL OUTLET COMP. (SHIFT DONE)
YFEED	-	CONVERTER INLET COMPOSITION VECTOR (MOLES/HR)
YINCR	-	VECTOR OF COMPOSITION CHANGES FOR DEW CHECK
YTOT	-	TOTAL MOLES IN STREAM PASSING THROUGH BED

A.4. CONDENSER

A.4.1 CONDENSER SIMULATION

$$XAREA = NTUBE * 3.14159 * DIAM**2 / (4 * 144)$$

$$GMAX = TMASS / (3600 * XAREA)$$

$$TINCR = 25.$$

A.4.2 CONDENSER DESIGN

$$XAREA = TMASS / (3600 * GMAX)$$

$$NTUBE = XAREA * 4 * 144 / (3.14159 * DIAM**2) + 0.5$$

$$TINCR = (TFEED - TOUT) / 10$$

A.4.3 SEGMENT CONDENSATE HEAT BALANCE EQUATION (REF. COUGHANOWR AND STENSHOLT(43))

$$QA1 = QA2 \quad \text{(MUST BE BALANCED BY ITERATIVELY GUESSING TCOND)}$$

$$QA1 = HG * (TMEAN - TCOND) * AC \\ + SULIQ * DELTA * AMWTS$$

$$HG = 0.023 * RE**(-0.2) * CPAVG * GAVG / PR**(2/3)$$

$$RE = GAVG * DIAM/12 / VIS$$

$$VIS = AVGMU * 2.42$$

$$GAVG = TMASS / (NTUBE * 3.14 * DIAM**2 / 4) * 144$$

$$PR = CPAVG * VIS / RK$$

$$RK = VIS * (CPAVG + 2.48 / AVMWTS) \\ \text{(REF. PERRY(47))}$$

$$AC = A / (1 - \exp(-A))$$

$$A = SULIQ * AMWTS * CPAVG / HG$$

$$SULIQ = RKG * (PPSUL - VPSUL)$$

$$RKG = RKGFC / PGF$$

$$RKGFC = HG * PR^{(2/3)} / (CPAVG * AVMWT * SC^{(2/3)})$$

$$PGF = (PPSUL - VPSUL) / \text{ALOG}((PRESS - VPSUL) / (PRESS - PPSUL))$$

$$SC = VIS / (RHO * DV)$$

$$DV = 0.0166 * TK32 * (1/AMWTS + 1/AMWTI)^{0.5} / (VSULF^{(1/3)} + VINRT^{(1/3)})^2 / PRESS / 14.7$$

$$TK32 = ((TFEED + TEMP) / 2 + 460) / 1.8^{1.5}$$

$$QA2 = UCTOS * (TCOND - TSTEM)$$

$$UCTOS = 1 / (1/HCOND + RSCWF)$$

$$HCOND = 327.8 * RELIQ^{(-1/3)} \quad (\text{REF. BENNETT AND MYERS(48)})$$

$$RELIQ = \tau * 0.1653$$

$$\tau = SFILM * 32 / (NTUBE * 3.14159 * DIAM/12)$$

$$ERROR = QA1 - QA2$$

A.4.4 CONDENSER SEGMENT LENGTH CALCULATION
(SEGMENT HEAT TRANSFER AREA ITERATIVELY CHOSEN TO SATISFY A TOTAL HEAT BALANCE ON THE SEGMENT)

$$QLOS1 = AREA * QA1$$

$$SMOLS = SULIQ * AREA$$

$$SLIQ = SMOLS * AMWTS / 32$$

$$SFOG1 = (SMINR - SMOLS) * AMWTS / 32$$

$$SFOG2 = 0.$$

$$SFOG = \text{MAX}(SFOG1, SFOG2)$$

$$SMINR = SULIN - SSAT$$

$$SSAT = VPMAX * YINRT / (PRESS - VPMAX)$$

$$QLOSS = \text{ENTHALPY}(SFOG + SLIQ + GAS)(\text{SEGMENT INLET}) - \text{ENTHALPY}(SFOG + SLIQ + GAS)(\text{SEGMENT OUTLET})$$

$$ERROR1 = QLOS1 - QLOSS$$

$$SGMTL = AREA / (NTUBE * 3.14159 * DIAM/12)$$

A.4.5 CONDENSER SEGMENT PRESSURE DROP

$$DP = DPPFT * SGM TL$$

$$DPPFT = 5 * GAVG^{**2} * FF / (DIAM * 1.E10 * RHO \\ * (AVGMU/WALMU)^{**0.14})$$

$$FF = 0.079 / RE^{**0.25}$$

$$RE = GAVG * DIAM/12 / VIS$$

A.4.6 PORTION OF LAST SEGMENT USED

FOR DESIGN,

$$RATIO = 1 + (TEMP' - TOUT) / TINC R$$

FOR SIMULATION,

$$RATIO = 1 - (TLONG + SGM TL - TLGTH) / SGM TL$$

A.4.7 TOTAL CONDENSER CONDENSATION AND RECOVERY

$$CRCOV = (SLIQ + SFOG) * 32 / TMSIN * 100$$

$$ARCOV = SLIQ * 32 / TMSIN * 100$$

A.4.8 RESULTING OVERALL CONDENSER HEAT TRANSFER COEFFICIENT
(NOT USED DIRECTLY IN THE ACTUAL CALCULATIONS)

$$UOVRL = QTOTL / ((DELT1 - DELT2)/ALOG(DELT1/DELT2) \\ * TAREA)$$

$$TAREA = NTUBE * 3.14159 * DIAM/12 * TLONG$$

$$DELT1 = TFEED' - TSTEM$$

$$DELT2 = TEMP' - TSTEM$$

NOMENCLATURE FOR SECTION A.4

AC	- ACKERMANN COEFFICIENT
AMWTI	- AVERAGE MOLECULAR WEIGHT OF INERT GAS
AMWTS	- AVERAGE MOLECULAR WEIGHT OF SULPHUR IN SEGMENT
ARCOV	- PERCENT RECOVERY OF INLET ELEMENTAL SULPHUR
AREA	- SEGMENT HEAT TRANSFER AREA (SQ.FT)
AVGMU	- GASEOUS VISCOSITY FOR SEGMENT (CP)
AVMWT	- AVERAGE MOLECULAR WEIGHT FOR TOTAL SEGMENT STREAM
CPAVG	- SEGMENT AVERAGE SPECIFIC HEAT (BTU/LB.DEG.F)
CRCOV	- PERCENT CONDENSATION OF INLET ELEMENTAL SULPHUR
DELTA	- SULPHUR LATENT HEAT OF VAPORIZATION (BTU/LB)
DIAM	- CONDENSER TUBE DIAMETER (INCHES)
DP	- PRESSURE DROP ACROSS WHOLE CONDENSER (PSIA)
DPPFT	- INCREMENTAL PRESSURE DROP THRU SEGMENT (PSI/FT)
DV	- DIFFUSIVITY OF S. VAPOR IN INERT GAS (LB/HR.SQ.FT)
FF	- FANNING FRICTION FACTOR
GAVG	- SEGMENT AVERAGE MASS VELOCITY (LB/HR.SQ.FT.)
GMAX	- MAX. CONDENSER MASS VELOCITY (LB/SEC.SQ.FT.)
HCOND	- HEAT TRANSFER COEFFICIENT FOR CONDENSATE FILM (BTU/HR.SQ.FT.DEG.F)
HG	- GAS SIDE HEAT TRANSFER COEFFICIENT FOR SEGMENT (BTU/HR.SQ.FT.DEG.F)
NTUBE	- NUMBER OF CONDENSER TUBES
PPSUL	- PARTIAL PRESSURE OF SULPHUR IN SEGMENT (PSIA)
PR	- SEGMENT PRANDL NUMBER
PRESS	- TOTAL PRESSURE IN SEGMENT (PSIA)
QA1	- HEAT TRANSFER RATE FROM GAS TO FILM (BTU/HR.SQ.FT)
QA2	- HEAT TRAN. RATE FROM FILM TO STEAM (BTU/HR.SQ.FT)
QLOS1	- SEG. HEAT LOSS BY HEAT AND MASS TRANSFER (BTU/HR)
QLOSS	- SEG. HEAT LOSS BY SEG. HEAT BALANCE (BTU/HR)
QTOTL	- TOTAL CONDENSER DUTY (BTU/HR)
RATIO	- FRACTION OF LAST CONDENSER SEGMENT USED.
RE	- SEGMENT REYNOLD NUMBER
RELIQ	- RENOLD NUMBER IN SULPHUR CONDENSATE FILM
RHO	- SEGMENT GAS DENSITY (LB/CU.FT.)
RK	- THERMAL CONDUCTIVITY OF SEG. GAS (BTU/HR.FT.DEG.F)
RKG	- CONVECTIVE MASS TRANSFER COEFFICIENT FOR SEGMENT (LB.MOLE.S./HR.SQ.FT.PSIA)
RSCWF	- (= 0.006) HEAT TRANSFER RESISTANCE FROM STEAM SIDE FOULING, CONDENSATE FOULING AND METAL WALL
SC	- SCHMIDT NUMBER FOR SEGMENT
SFILM	- TOTAL ACCUMULATED SULPHUR COND. FILM (MOLES/HR)
SFOG	- MOLES SULPHUR FOG FORMED IN SEGMENT
SGMTL	- CALCULATED LENGTH OF CONDENSER SEGMENT (FT)
SLIQ	- MOLES SULPHUR LIQUID (TO FILM) IN SEGMENT
SMINR	- MINIMUM SULPHUR REMOVAL TO PREVENT SUPER-COOLING AT SEGMENT OUTLET (LB.MOLE.S/HR)
SMOLS	- MOLES SULPHUR TO FILM IN SEGMENT (LB.MOLE/HR)
SSAT	- MOLES SULPHUR (AT SATURATION) AT SEG. OUTLET TEMP.
SULIQ	- SEGMENT MASS TRANSFER RATE (LB.MOLE.S/HR.SQ.FT)

TAREA	-	TOTAL CONDENSER HEAT TRANSFER AREA (SQ.FT)
TCOND	-	SULPHUR CONDENSATE FILM TEMP. FOR SEGMENT (DEG.F)
TEMP	-	CONDENSER SEGMENT OUTLET TEMPERATURE (DEG.F)
TEMP'	-	CONDENSER GAS OUTLET TEMPERATURE (DEG.F)
TFEED	-	CONDENSER SEGMENT INLET TEMPERATURE (DEG.F)
TFEED'	-	CONDENSER FEED TEMPERATURE (DEG.F)
TINCR	-	TEMP. INCREMENT DEFINING A CONDENSER SEGMENT (DEG.F)
TLGTH	-	SPECIFIED CONDENSER TUBE LENGTH (FT)
TLONG	-	TOTAL ACCUMULATED CONDENSER SEGMENT LENGTHS (FT)
TMASS	-	TOTAL MASS OF STREAM THRU CONDENSER TUBES (LB/HR)
TMEAN	-	MEAN BULK GAS TEMPERATURE FOR SEGMENT (DEG.F)
TMSIN	-	TOTAL MASS OF INLET ELEMENTAL SULPHUR (LB/HR)
TOUT	-	SPECIFIED CONDENSER OUTLET TEMPERATURE (DEG.F)
TSTEM	-	SHELL SIDE STEAM TEMPERATURE (SATURATED) (DEG.F)
UCTOS	-	OVERALL H.T. COEFFICIENT FOR CONDENSATE TO STEAM (BTU/HR.SQ.FT.DEG.F)
UOVRL	-	CONDENSER OVERALL HEAT TRANSFER COEFFICIENT (BTU/HR.SQ.FT.DEG.F)
VINRT	-	AVE. MOLECULAR VOLUME OF INERT GAS IN SEGMENT
VIS	-	GASEOUS VISCOSITY FOR SEGMENT (LB/FT.HR.)
VPMAX	-	SULPHUR VAPOR PRESS. AT SEG. OUTLET TEMP. (PSIA)
VPSUL	-	VAPOR PRESS. OF SULPHUR AT SEG. COND. TEMP. (PSIA)
VSULF	-	AVERAGE MOLECULAR VOLUME OF S. VAPOR IN SEGMENT
XAREA	-	TOTAL TUBE CROSS-SECTIONAL AREA FOR FLOW (SQ.FT.)
YINRT	-	TOTAL MOLES OF INERT GAS IN SEGMENT (MOLES/HR)

A.5. ADIABATIC STREAM COMBINER

A.5.1 ITERATIVE DETERMINATION OF A NEW STREAM SPLIT IF AN INFORMATION RECYCLE STREAM EXISTS

$$YCOMP(I) = YFED2(I) * (1 - EPS) / (1 - EPSTR) + YFED1(I) * EPS / EPSTR$$

$$ENTHR = ENTH1 * EPS / EPSTR + ENTH2 * (1 - EPS) / (1 - EPSTR)$$

$$TCALC = FCN(ENTHR, YCOMP')$$

$$ERROR = TDSIR - TCALC$$

NOMENCLATURE FOR SECTION A.5

ENTHR	-	TOTAL INLET ENTHALPY FOR ESTIMATED STREAM SPLIT
ENTH1	-	ENTHALPY OF GIVEN HOT STREAM
ENTH2	-	ENTHALPY OF GIVEN COLD STREAM
EPS	-	ESTIMATED VALUE OF PRECEEDING EQUIPMENT STREAM SPLIT WHICH WILL YIELD DESIRED OUTLET TEMPERATURE
EPSTR	-	GIVEN (INITIAL OR PREVIOUS) STREAM SPLIT
TCALC	-	TEMP. RESULTING FROM ESTIMATED INLET STREAMS
TDSIR	-	DESIRED COMBINER OUTLET TEMPERATURE (DEG.F)
YCOMP	-	VECTOR OF MOLE NUMBERS TO EQUILIBRIUM CALCULATION
YCOMP'	-	COMPOSITION (SULPHUR SHIFT) RESULTING FROM ESTIMATED INLET STREAMS
YFED1	-	VECTOR OF MOLE NUMBERS FOR HOT INLET STREAM
YFED2	-	VECTOR OF MOLE NUMBERS FOR COLD INLET STREAM

A.6. STREAM COMBINER/DIVIDER

A.6.1 ITERATIVE DETERMINATION OF RESULTING TEMPERATURE FOR
STREAM COMBINING - NEWTON'S METHOD IS USED. (THIS
PROCEDURE IS USED FOR ALL EQUIPMENT WITH MULTIPLE
FEEDS)

$T_{NEW} = T_{OLD} - \text{ERROR} / DHDT$

$DHDT = CP * Y_{TOT}$

$\text{ERROR} = ENTH - ENTHR$

$RELER = \text{ERROR} / ENTHR$

NOMENCLATURE FOR SECTION A.6

- | | | |
|-------|---|--|
| CP | - | STREAM HEAT CAPACITY (FIRST DERIVATIVE OF MOLAL ENTHALPT W.R.T. TEMPERATURE) (BTU/LB.MOLE.DEG.F) |
| DHDT | - | DERIVATIVE OF TOTAL ENTHALPY W.R.T. TEMPERATURE (BTU/DEG.F) |
| ENTH | - | STREAM ENTHALPY CORRESPONDING TO TOLD (BTU/HR) |
| ENTHR | - | ACTUAL (REFERENCE) STREAM ENTHALPY (BTU/HR) |
| RELER | - | RELATIVE ERROR - MUST BECOME LESS THAN SOME CRITERION BEFORE ITERATION IS DISCONTINUED |
| TOLD | - | LAST ESTIMATE OF CORRECT TEMPERATURE |
| TNEW | - | NEW ESTIMATE OF CORRECT TEMPERATURE |
| YTOT | - | TOTAL MOLES IN STREAM |

A.7. COMBUSTION AIR ADDER

A.7.1 CALCULATION OF AIR STREAM TO BE ADDED

$$\begin{aligned} \text{YAIR}(\text{NO}_2) = & \text{SPEC1} * 0.5 * (\text{SUMS}(1) * 2 * \text{SPEC2} \\ & + \text{SUMS}(3) * 2 + (\text{SUMS}(4) - 2 * \text{SUMS}(1) \\ & * (1 - \text{SPEC2})) * 0.5 - \text{SUMS}(2)) \end{aligned}$$

$$\text{YAIR}(\text{NN}_2) = \text{YAIR}(\text{NO}_2) * 79 / 21$$

$$\text{VPH2O}' = \text{VPH2O} * 14.7 * \text{RELHY} / 100$$

$$\begin{aligned} \text{YAIR}(\text{IDH}_2\text{O}) = & \text{VPH2O}' * (\text{YAIR}(\text{NO}_2) + \text{YAIR}(\text{NN}_2)) \\ & / (\text{PAIR} - \text{VPH2O}') \end{aligned}$$

NOMENCLATURE FOR SECTION A.7

PAIR	-	TOTAL PRESSURE OF AIR STREAM (PSIA)
RELHY	-	RELATIVE HUMIDITY OF AIR STREAM (PERCENT)
SPEC1	-	EXCESS OR DEFICIENT AIR COEFFICIENT
SPEC2	-	FRACTION OF SULPHUR (AS H ₂ S) TO BE BURNED
SUMS(1)	-	TOTAL ATOMS OF SULPHUR IN ACID GAS FEED
SUMS(2)	-	TOTAL ATOMS OF OXYGEN IN ACID GAS FEED
SUMS(3)	-	TOTAL ATOMS OF CARBON IN ACID GAS STREAM
SUMS(4)	-	TOTAL ATOMS OF HYDROGEN IN ACID GAS FEED
YAIR(NN ₂)	-	AIR STREAM NITROGEN MOLE NUMBER (MOLES/HR)
YAIR(NO ₂)	-	AIR STREAM OXYGEN MOLE NUMBER (MOLES/HR)
YAIR(IDH ₂ O)	-	AIR STREAM WATER MOLE NUMBER (MOLES/HR)
VPH2O	-	VAPOR PRESS. OF WATER AT AIR TEMPERATURE (PSIA)
VPH2O'	-	PARTIAL PRESSURE OF WATER IN AIR STREAM (PSIA)

A.8. INCINERATOR

A.8.1 CALCULATION OF AIR AND FUEL AND AIR STREAMS (ITERATIVE CALCULATION OF FUEL FOR DESIGN CASE)

$$YCOMP(I) = YFEED(I) + YGAS(I) * FACTR$$

$$ENTHR = ENTH1 + ENTH2 * FACTR$$

$$ENTHN = ENTHALPY (EQUIL. COMP. AT DESIRED TEMP.)$$

$$ERROR = ENTHN - ENTHR$$

NOMENCLATURE FOR SECTION A.8

ENTHN	-	ENTHALPY OF EQUILIBRIUM COMPOSITION (AT DESIRED INCINERATOR OUTLET TEMPERATURE) RESULTING FROM AIR AND FUEL GAS STREAM ESTIMATE.
ENTHR	-	TOTAL INLET ENTHALPY (FOR PRESENT AIR AND GAS INLET ESTIMATE).
ENTH1	-	ENTHALPY OF INLET PROCESS GAS (+ AIR)
ENTH2	-	ENTHALPY OF INLET FUEL GAS SAMPLE (+AIR)
FACTR	-	ESTIMATE OF FUEL SAMPLE MULTIPLIER REQUIRED
YCOMP	-	VECTOR OF MOLE NUMBERS TO EQUILIBRIUM CALCULATION
YFEED	-	VECTOR OF MOLE NUMBERS OF INLET PROCESS GAS AND AIR (TO BURN PROCESS GAS + SPECIFIED EXCESS)
YGAS	-	VECTOR OF MOLE NUMBERS OF FUEL GAS (SAMPLE COMP.) AND AIR (TO BURN SAMPLE + SPECIFIED EXCESS)

A.9. STACK

A.9.1 CALCULATION OF MAX. GROUND CONCENTRATION (SIMULATION)

$$C_{MAX} = PROD / ESH^{**2}$$

$$ESH = HSTAK + 0.75 * (VRISE + TRISE)$$

A.9.2 CALCULATION OF REQUIRED STACK HEIGHT (DESIGN)

$$HSTAK = ESH - (VRISE + TRISE) * 0.75$$

$$ESH = (PROD / C_{MAX})^{**0.5}$$

$$PROD = 2.35E5 * QSO2 * AMU(WVEL)$$

-- VELOCITY RISE CALCULATION

$$VRISE = 4.77 / (1 + 0.43 * WVEL/VSTAK) * SQQV / WVEL$$

$$SQQV = (QTOT * VSTAK)^{**0.5}$$

$$VSTAK = 4 * QTOT / (3.14159 * DIAM^{**2})$$

-- TEMPERATURE RISE CALCULATION

$$TRISE = 6.37 * 32.17 * QTOT * DELT * Z / (TRANK * WVEL^{**3})$$

$$DELT = TSTAK - TEQIV$$

$$TEQIV = TMASS / YTOT / 29 * TAMB$$

$$QTOT = YTOT * FACTR$$

$$QSO2 = YFEED(ISO2) * FACTR$$

$$FACTR = 10.73 * (TEQIV + 460) / (PRESS * 3600)$$

$$TRANK = TEQIV + 460$$

-- CALCULATION OF FACTOR Z

- MODERATELY STABLE ATMOSPHERIC CONDITIONS

$$Z = ALOG(J^{**2}) + 2 / J - 2$$

$$J = WVEL^{**2} / SQQV * (SQR - 0.28 * VSTAK * TRANK / (32.17 * DELT)) + 1$$

$$SQR = GFACT(WVEL) * TRANK**0.5$$

- MODERATELY UNSTABLE ATMOSPHERIC CONDITIONS

$$XB = DISTX * WVEL / (3.57 * SQQV) \quad (ITERATIVE)$$

$$XB \quad 20, \quad Z = (ALOG(XB) / 2.303 - 0.3553) / 0.2286$$

$$XB \quad 20, \quad Z = XB / (2.172 + 0.1359 * XB)$$

$$DISTX = 10 * ESH$$

$$ESH = HSTAK + 0.75 * (VRISE + TRISE)$$

$$WVMIN = (32.17 * DELT / TRANK * (QTOT / VSTAK)**0.5)**0.5$$

A.9.3 DISTANCE TO MAXIMUM GROUND CONCENTRATION

$$DIST = 20 * ESH \quad (STABLE)$$

$$DIST = 10 * ESH \quad (UNSTABLE)$$

NOMENCLATURE FOR SECTION A.9

AMU	-	A FUNCTION OF WIND VELOCITY
CMAx	-	MAXIMUM GROUND CONCENTRATION (PPM)
DIST	-	DISTANCE TO MAXIMUM GROUND CONCENTRATION (FT)
ESH	-	EFFECTIVE STACK HEIGHT (FT)
GFACT	-	A FUNCTION OF WIND VELOCITY
HSTAK	-	ACTUAL STACK HEIGHT (FT)
ISO2	-	SPECIE NUMBER OF SO2 COMPONENT
PRESS	-	STACK INLET STREAM PRESSURE (PSIA)
QSO2	-	VOLUMETRIC FLOWRATE OF SO2 (CU.FT./SEC)
QTOT	-	TOTAL VOLUME OF INLET GAS (CU.FT./SEC)
TAMBI	-	AMBIENT AIR TEMPERATURE (DEG.F)
TEQIV	-	TEMPERATURE AT WHICH STACK GAS DENSITY EQUALS THAT OF THE AMBIENT AIR (DEG.F)
TMASS	-	TOTAL MASS OF STACK INLET STREAM (LB/HR)
TRISE	-	STACK GAS TEMPERATURE RISE DUE TO BOUYANCY (FT)
TSTAK	-	STACK GAS TEMPERATURE EXIT STACK (DEG.F)
VSTAK	-	VELOCITY OF GAS OUT OF STACK (FT/SEC)
VRISE	-	STACK GAS VELOCITY RISE DUE TO MOMENTUM (FT)
WVEL	-	WIND VELOCITY (FT/SEC)
WVMIN	-	MINIMUM WIND VELOCITY FOR WHICH UNSTABLE CALCULATIONS ARE VALID (FT/SEC)
YFEED	-	VECTOR OF STACK INLET STREAM MOLE NUMBERS
YTOT	-	TOTAL MOLES IN STACK INLET STREAM

A.10. MISCELLANEOUS -----

A.10.1 DEW POINT CALCULATION

-- WATER

$$YFRAC = Y(IDH2O) / YTOT$$

-- SULPHUR (TEMP BELOW 700 F)

$$YFRAC = STOT / YTOT$$

-- SULPHUR (TEMP ABOVE 700 F)
(CONVERT ALL SULPHUR TO S8 FORM)

$$YFRAC = S_{MASS} / (32 * 8) / YTOT$$

NEWTON'S METHOD IS USED TO CONVERGE TO THE DEW POINT
TEMPERATURE SUCH THAT -

$$PARTP = PCALC(TF)$$

$$PARTP = PRESS / 14.7 * YFRAC$$

A.10.2 VAPOR PRESSURE CALCULATION

-- WATER (REF. KEENAN AND KEYS(49))

$$PCALC = 218.167 * \exp(-2.303 * (V * U / W))$$

$$V = X / TK$$

$$U = 3.3463130 + 4.14113E-2 * X + 7.515484E-9 * X**3 \\ + 6.56444E-11 * X**4$$

$$W = 1 + 1.379448E-2 * X$$

$$X = 647.27 - TK$$

$$TK = (TF + 460) / 1.8$$

-- SULPHUR (REF. TEXAS GULF SULPHUR DATA(50))

- FOR TK LESS THAN 600 DEG. K.

$$PCALC = \exp((14.7 - 0.0062238 * TK - 5405.1 / TK) \\ * 2.303) / 760.$$

- FOR TK GREATER THAN 600 DEG. K,

$$PCALC = \exp((7.43287 - 3268.2/TK) * 2.303) / 760.$$

A.10.3 STEAM PRODUCTION

$$PRODM = PROD / WTMOL(IDH2O)$$

$$PROD = DUTY / CDELH$$

$$CDELH = DELHV + COREC$$

$$DELHV = \exp(7.0095 + 0.3542 * \text{ALOG}(1 - TSTEM/705.4))$$

$$COREC = TSTEM - TSIN$$

NOMENCLATURE FOR SECTION A.10

CDELH	-	CORRECTED LATENT HEAT OF VAPORIZATION (H2O,BTU/LB)
COREC	-	LATENT HEAT CORRECTION (LB/HR)
DELHV	-	LATENT HEAT OF VAPORIZATION OF WATER (BTU/LB)
DUTY	-	EQUIPMENT DUTY OR TOTAL HEAT LOAD (BTU/HR)
IDH2O	-	WATER VAPOR SPECIE
PARTP	-	PARTIAL PRESSURE OF WATER OR SULPHUR (ATM.)
PCALC	-	CALCULATED VAPOR PRESSURE AT GUESSED TEMP. (ATM.)
PRESS	-	TOTAL PRESSURE OF STREAM (PSIA)
PROD	-	STEAM PRODUCTION (LB.H2O/HR.)
PRODM	-	STEAM PRODUCTION (LB.MOLES H2O/HR.)
SMASS	-	TOTAL POUNDS OF SULPHUR IN STREAM
STOT	-	TOTAL MOLES OF SULPHUR VAPOR IN STREAM
TF	-	ESTIMATED DEW POINT TEMPERATURE (DEG.F)
TK	-	TEMPERATURE (DEG.K)
TSIN	-	FEED-WATER INLET TEMPERATURE (DEG.F)
TSTEM	-	SATURATION TEMPERATURE OF STEAM
YFRAC	-	MOLE FRACTION OF WATER OR SULPHUR
YTOT	-	TOTAL MOLES IN STREAM OF INTEREST
Y(IDH2O)	-	TOTAL MOLES OF WATER VAPOR IN STREAM
WTMOL	-	VECTOR OF SPECIE MOLECULAR WEIGHTS

APPENDIX B

THIS APPENDIX CONTAINS SEVERAL EXAMPLE DATA SETS AND ALSO, THE DEFINITIONS OF THE EQUIPMENT PARAMETERS FOR THE EQUIPMENT MODULES DEVELOPED.

EXAMPLE DATA SETS

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B.3. MOLECULAR AND THERMODYNAMIC DATA B-4

B.4. EQUIPMENT PARAMETER SPECIFICATIONS AND ESTIMATES . B-5

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B.8. EXAMPLE DATA ILLUSTRATING INFORMATION RECYCLE . . B-9

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TABLE B-2 IN-LINE BURNER EQUIPMENT PARAMETERS B-14

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TABLE B-9 EFFLUENT STACK EQUIPMENT PARAMETERS B-21

B.1. EXAMPLE OF SEVERAL EQUIVALENT DATA SETS

DESIRED INPUT -
 INTEGERS - 1, -17, 1950
 REALS - -6., 157200., 62.317
 ALPHAMERICS - A, B, C

1, -17, 1950, -6., 157200., 62.317 'ABC' **

1 -6. -17 'A' 'B' 1950 157200. 62.317 'C' **

'A'	1,	-6.	C	FIRST CARD
'B'	-17	1.572E5	C	SECOND CARD
'C'	1950	.62317E2	C	THIRD CARD
**			C	FOURTH CARD

'A', 1, -6. 'B' -17 +1572E+2
 'C' 1950 62317E-3 **

1, -17, 1950	C	USE AS MANY CARDS
-6. 157200.0 62.3170	C	AS YOU WANT AND
'A' 'B', 'C' **	C	USE COMMENTS.

B.2. EXAMPLE DATA SET USING DATA CONTROL MESSAGES

EXAMPLE SECTION	C	SECTION BEGINS.
1,2,3 **	C	CONTROL RETURNED TO CALLING
1.,6.,7 **	C	ROUTINE AT END OF EACH DATA
'EXAMPLE' 3 **	C	SEGMENT - END OF SEGMENT
55.,54.,53.0 '52'	C	INDICATED BY **
1 2 3 4 5 6	C	SEGMENTS MAY VARY IN LENGTH.
7 8 9 10 11 **		
END	C	SECTION ENDS
NEXT SECTION **		
1,2,3 **		
7 8 9 *END*	C	*END* IMPLIES **
LAST SECTION 1,2,3		*END OF ALL DATA*

B.3. MOLECULAR AND THERMODYNAMIC DATA

LOGICAL EXAMPLE

```

*MOLECULAR AND THERMODYNAMIC DATA*
ISYMB,ATMWT,VATOM,  ISYMB,ATMWT,VATOM  ....
          ....  ISYMB,ATMWT,VATOM  **
NAME,PHASE,V(1),V(2),A(1)  ...  A(14)  **
NAME,PHASE,V(1),V(2),A(1)  ...  A(14)  **
          .....
          .....
*END*

```

NUMERICAL EXAMPLES

```

*MOLECULAR AND THERMODYNAMIC DATA*
'H' 1. 3.7      C      ATOM SYMBOL, WEIGHT, VOLUME
'C' 12. 14.8      'O' 16. 7.4
'S' 32. 25.6      'N' 14. 15.6  **
'H2O ' 0.008 0.000021      C VISCOSITY GIVEN.
1. 2. 3. 4. 5. 6. 7.      C FICTIONAL THERMODYNAMIC
8. 9. 10. 11. 12. 13. 14.  **      C COEFFICIENTS
'SO2 ' 'G'      C PHASE GIVEN.
1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 11. 12. 13. 14.  **
'S      'L'      C LIQUID SULPHUR
1.,2.,3.,4.,5.,6.,7.,8.,9.,10.,11.,12.,13.,14.**'S2 '
1.,2.,3.,4.,5.,6.,7., 8.,9.,10.,11.,12.,13.,14.,
*END*

```

```

*MOLECULAR AND THERMODYNAMIC DATA*
'HCOSEN'      C ATOM TYPES
1. 3.7, 12. 14.8, 16. 7.4, 32. 25.6, 14. 15.6
C      WEIGHT,VOLUME,WEIGHT,VOLUME.....
**  'H2O G'      0.008,0.000021,
+4.1565016E+00 -1.7244334E-03 +5.6982316E-06
-4.5930044E-09 +1.4233654E-12 -3.0288770E+04
-6.8616246E-01      C      LOW TEMPERATURE
2.6707532E+00 +3.0317115E-03 -8.5351570E-07
+1.1790853E-10 -6.1973568E-15 -2.9888994E+04
+6.8838391E+00      C      HIGH TEMPERATURE
**
.....
.....
*END*

```


B.4. EQUIPMENT PARAMETER SPECIFICATIONS AND ESTIMATES

LOGICAL EXAMPLES

```
*EQUIPMENT PARAMETER SPECIFICATIONS*
INUMB, ITYPE,  INUMB, ITYPE,  .....  INUMB, ITYPE  **
IEQIP,  IPAR, VALUE,  IPAR, VALUE,  ....  IPAR, VALUE  **
IEQIP,  IPAR, VALUE,  IPAR, VALUE,  ....  IPAR, VALUE  **
```

```
.....
.....
```

```
*END*
```

```
*EQUIPMENT PARAMETER ESTIMATES*
IEQIP,  IPAR, VALUE,  IPAR, VALUE,  ....  IPAR, VALUE  **
IEQIP,  IPAR, VALUE,  IPAR, VALUE,  ....  IPAR, VALUE  **
```

```
.....
.....
```

```
*END*
```

NUMERICAL EXAMPLES

```
*EQUIPMENT PARAMETER SPECIFICATIONS*
17 1, 3 4, 6 3  **
C  NO. 17 = WASTE HEAT BOILER,      NO. 3 = CONDENSER
C  NO. 6 = CONVERTER
  3      C  EQUIP. NO. 3 (CONDENSER SIMULATION SPECS.)
1 1.      C  CONDENSER NUMBER = 1
2 20.      C  TUBE LENGTH = 20. FEET
3 1.5      C  TUBE DIAMETER = 1.5 INCHES
4 1000.      C  1000 TUBES
5 50.      C  STEAM PRESSURE = 50 PSIA.
7 12.      C  SULPHUR OUTLET STREAM = NO. 12
10 10.** C  MAXIMUM OUTLET FOG = 10 LB/100 MOLES GAS
C  WASTE HEAT BOILER DESIGN SPECS.
17 1 3., 3 1., 10 900., 11 600., 13 0.5, 14 .5,
    15 0.6, 19 0.2, 20 7.  **
C  CONVERTER DESIGN SPECS.
6 1 1. 6 1. 7 2.97 8 0.25  *END*
```

```
C
*EQUIPMENT PARAMETER ESTIMATES*
17      C  ESTIMATES FOR WASTE HEAT BOILER
26 1990.  C  ESTIMATE OF ADIABATIC FLAME TEMP.
5 250. *END*  C  ESTIMATE OF 3RD PASS TUBE NUMBER
```

```
*EQUIPMENT PARAMETER SPECIFICATIONS*
C  SINGLE STACK SIMULATION  -  COMPLETE JOB.
1 9** 1 1 70. 2 1200. 3 250. 4 3.5  *END*
```


B.5. STREAM SPECIFICATIONS AND ESTIMATES

LOGICAL EXAMPLE

```

*STREAM SPECIFICATIONS*      (OR *STREAM ESTIMATES* )
ISTRM,  IPAR,VALUE,  IPAR,VALUE  ....  IPAR,VALUE  **
          ***** OR *****
ISTRM    VALUE,VALUE,VALUE,VALUE  ....VALUE  **

ISTRM,  IPAR,VALUE,  IPAR,VALUE  ....  IPAR,VALUE  **
          ***** OR *****
ISTRM    VALUE,VALUE,VALUE,VALUE  ....VALUE  **
          .....
          .....
*END*

```

NUMERICAL EXAMPLE

```

*STREAM SPECIFICATIONS*
C      MOLE NUMBERS NOT SPECIFIED ARE ASSUMED ZERO.
1      1 1.5677  2 104.2917  5 47.  6 290.0417
      21 70.  22 14.7 **      C STREAM NUMBER 1
C      1ST, 2ND, 5TH, AND 6TH MOLE NUMBERS SPECIFIED
C      - ALSO TEMPERATURE AND PRESSURE.
2      22 14.7  21 70.0 **
C      STREAM NO. 2 - TEMP. AND PRESS. SPECS ONLY.
14     0.  105.25632  0.  556.95703  246.87311
      92.57214  46.83867  0.  8E-5  0.08824  0.39
      0.41704  66E-5  0.73039  .13123  4.92082
      314.2  14.15 **
C      FOR STREAM 14, ALL 16 MOLE NUMBERS SPECIFIED,
C      ALSO TEMP. AND PRESS. (LAST TWO).
C      NOTE - FOR THIS JOB, 18 REAL VALUES MUST BE GIVEN
C              FOR ALL STREAMS IF IPAR IS NOT USED.
C              ALSO - VALUES MUST BE IN CORRECT ORDER.
9      5 865.4  4 1847.05  3 35.14  2 345.85  7 37.
      21 1200.  22 12.2 **      C NOTE ARBITRARY ORDER OF
C              PARAMETER VALUES IF IPAR'S ARE USED.
*END*      *STREAM ESTIMATES*
40 1 .1 **      C INFORMATION STREAM NO. 40 ESTIMATE.
C      (INITIAL STREAM SPLIT ESTIMATE)
C      IPAR SHOULD ALWAYS BE USED FOR INFORMATION
C      STREAM SPECIFICATIONS OR ESTIMATES.
17     1 20.  21 100.  22 12.2 *END*
C      SAMPLE COMPOSITION, TEMP. AND PRESS. FOR
C      INCINERATOR FUEL GAS STREAM (STREAM NO. 17)

```


B.6. FLOWSHEET DATA

LOGICAL EXAMPLE

```
*FLOWSHEET DATA*
ISTRM,IFROM,ITO,IUNKN,IFLAG **
ISTRM,IFROM,ITO,IUNKN,IFLAG **
      .....
      .....
```

NUMERICAL EXAMPLES

```
*FLOWSHEET DATA*
1 0 1** 2 0 1** 3 1 2 4** 4 2 3** 5 2 4** 6 4 5**
7 3 6** 8 5 7 2** 9 6 5** 10 6 0** 11 7 0** 12 0 8**
13 0 8** 14 8 9** 15 0 3 0 1** 16 3 1 1 1**
40 3 1 +1 -1**          *END*
```

```
*FLOWSHEET DATA*
1 0 1**      C      ACID GAS TO BOILER
2 0 1**      C      AIR TO BOILER
3 1 2 10**   C      BOILER DISCHARGE TO FIRST CONDENSER
4 1 3 9**    C      BOILER HOT GAS BYPASS TO REHEATER
36 3 1 1 -1** C      BOILER SPLIT INFORMATION FEED-BACK
5 2 3 10**   C      CONDENSER TO REHEATER
6 3 4**      C      REHEATER TO CONVERTER
7 5 6**      C      CONDENSER NO. 2 TO INCINERATOR
18 4 5**     C      CONVERTER TO CONDENSER
8 6 7**      C      INCINERATOR TO STACK
10 2 0**     C      SULPHUR PRODUCT FROM COND. NO. 1
11 5 0**     C      SULPHUR PROD. FROM COND. NO. 2
9 7 0 5 0**  C      STACK VENT TO ATMOSHERE.
27 0 1 1 1** C      BOILER FEED WATER.
28 1 0 2 1** C      BOILER PRODUCT STEAM.
*END*
```


B.7. PROGRAM CONTROL PARAMETERS

LOGICAL EXAMPLE

```
*PROGRAM CONTROL PARAMETERS*
IDBUG(1),IDBUG(2),.....IDBUG(15)
CRIT, 'NO OPTIMIZATION'    'PRINT SUPPRESS' *END*
```

NUMERICAL EXAMPLES

```
*PROGRAM CONTROL PARAMETERS*
 1 1 2 1 3 1 4 1 1 0 0 0 0 2 1 , 1E-3
'PRINT SUPPRESS'      *   E   N   D   *
C      DEFINING ALL ELEMENTS OF IDBUG, AND CRIT
```

```
*PROGRAM CONTROL PARAMETERS*    **
1 2 1 1 1 1 1 1 1 'NO OPTIMIZATION' *END*
C      DEFINING FIRST NINE ELEMENTS OF IDBUG
```


B.8. EXAMPLE DATA (ILLUSTRATING INFORMATION RECYCLE) -----

FLOWSHEET DATA

1	0	1		C	FEED TO STREAM DIVIDER
2	1	2		C	DIVIDER TO W.H.B.
10	2	4		C	BOILER BYPASS TO COMBINER 1.
40	4	2	1 -1	C	INFORMATION FROM COMBINER 1. TO BOILER
				C	(RE STREAM SPLIT)
11	1	3		C	DIVIDER TO IN-LINE BURNER
12	3	5		C	IN-LINE BURNER TO COMBINER 2.
41	5	1	1 -1	C	INFORMATION FROM COMBINER 2. TO SPLITTER
				C	(RE BOILER BYPASS)
30	8	4		C	CONDENSER 1. TO COMBINER 1.
31	9	5		C	CONDENSER 2. TO COMBINER 2.

...
...

END *EQUIPMENT PARAMETER SPECIFICATIONS*

1	6,		C	STREAM SPLITTER
2	1,		C	WASTE HEAT BOILER
3	2,		C	IN-LINE BURNER
4	5,		C	ADIABATIC STREAM COMBINER 1.
5	5,		C	ADIABATIC STREAM COMBINER 2.

...
...

1	1	0.05	**	C	STREAM DIVIDER SPLIT ESTIMATE AS
				C	EQUIPMENT PARAMETER SPECIFICATION.

...
...

END *STREAM SPECIFICATIONS*

...
...

40				C	INFORMATION STREAM 40
1	1.	**		C	STREAM PARAMETER 1 - DESTINATION OF
				C	INFORMATION TO DIVIDER - STREAM
				C	SPLIT - EQUIP. PAR. NO. 1.
41				C	INFORMATION STREAM 41
1	19			C	STREAM PARAMETER 1 - DESTINATION OF
				C	INFORMATION TO BOILER - BYPASS NO. 1
				C	EQUIP. PAR. NO. 19.
2	12.	**		C	PARAMETER 2 - INITIAL ESTIMATE OF
				C	NO. 1 BOILER BYPASS (12 PERCENT)

...
...

END OF ALL DATA

B.9. NOTES ON INFORMATION STREAMS AND RECYCLE

1. - THE FLOWSHEET DATA RELATED TO INFORMATION STREAMS SPECIFIES THE EQUIPMENT SOURCE AND EQUIPMENT DESTINATION OF THE INFORMATION CONVEYED BY THE INFORMATION STREAM.
(EG.) 40 1 2 1 -1
 INFORMATION STREAM 40 CONVEYS 1 PIECE OF INFORMATION FROM EQUIPMENT NO. 1 TO EQUIPMENT NO. 2
(ADDITIONAL INFORMATION REGARDING THE SPECIFIC DESTINATION OF THE INFORMATION IS REQUIRED.)
2. - THE STREAM PARAMETERS ASSOCIATED WITH INFORMATION STREAMS DO NOT HAVE THE SAME SIGNIFICANCE AS THE PARAMETERS OF A NORMAL STREAM (IE. 1 - 20 MOLE NUMBERS, 21 TEMPERATURE AND 22 PRESSURE)
THE SIGNIFICANCE OF THE INFORMATION STREAM PARAMETERS IS AS FOLLOWS -
PARAMETER NO'S 1 (,3,5) - THE EQUIPMENT STREAM PARAMETER NUMBER(S) OF THE DESTINATION EQUIPMENT TO WHICH INFORMATION IS BEING CONVEYED.
PARAMETER NO'S 2 (,4,6) - THE VALUE(S) OF THE ABOVE EQUIPMENT PARAMETER(S) (IE. THE INFORMATION)
PARAMETER NO'S (7,....,22) - NOT USED.
3. - THE DESTINATION LOCATIONS OF THE INFORMATION (EQUIPMENT PARAMETER NUMBER(S)) MUST BE SPECIFIED AS STREAM SPECIFICATIONS FOR THE INFORMATION STREAM.
(INITIAL ESTIMATES OF THE EQUIPMENT PARAMETER VALUES BEING CONVEYED MAY ALSO BE SPECIFIED AS INFORMATION STREAM SPECIFICATIONS, RATHER THAN THE CORRESPONDING EQUIPMENT PARAMETER ESTIMATES)
4. - THE EQUIPMENT MODULE WHICH IS THE SOURCE OF THE INFORMATION MUST BE SPECIFICALLY PROGRAMMED TO INSERT THE FEED-BACK INFORMATION AS THE APPROPRIATE PARAMETERS IN THE INFORMATION STREAM. HOWEVER, NO SUCH PROGRAMMING IS REQUIRED FOR THE MODULE WHICH IS THE DESTINATION OF THE INFORMATION STREAM - THE EXECUTIVE COMPLETES THIS FUNCTION WHEN RECYCLE OF CALCULATIONS OCCURS.
(NOTE THAT ONLY ONE, TWO, OR THREE AT MOST 'PIECES' OF INFORMATION MAY BE CONVEYED BY A SINGLE INFORMATION STREAM.)

LEGEND FOR TABLES B-1 TO B-9

- CM - CONDITIONALLY MANDATORY SPECIFICATION - REQUIRED UNDER CERTAIN CIRCUMSTANCES (REFERENCE NOTES).
- DES. - SPECIFICATIONS (AND ESTIMATES) REQUIRED OR PERMISSIBLE FOR THE DESIGN CASE.
- MS - MANDATORY SPECIFICATION - ALWAYS A NECESSARY SPECIFICATION FOR THE INDICATED MODE (DESIGN OR SIMULATION).
- NOTE - REFERENCES TO NOTES BELOW THE TABLE
- OE - OPTIONAL ESTIMATE - IF GIVEN, WILL BE USED AS AN INITIAL GUESS. A GOOD ESTIMATE FOR THE VALUES SHOWN MAY BE USED TO REDUCE THE COMPUTATION REQUIRED TO ACHIEVE CONVERGENCE.
- OS - OPTIONAL SPECIFICATION - MAY BE GIVEN IF DESIRED. IF NOT GIVEN, INDICATED VALUE IS ASSUMED.
- P.N. - EQUIPMENT PARAMETER NUMBER
- SIM. - SPECIFICATIONS (AND ESTIMATES) REQUIRED OR PERMISSIBLE FOR THE SIMULATION CASE.
- VALUE - VALUE OF THE PARAMETER WHICH IS ASSUMED BY THE MODULE IF REQUIRED FOR THE CALCULATIONS, BUT NOT SPECIFIED. (ONLY VALUES FOR THOSE PARAMETERS SHOWN ARE ASSUMED IF NEEDED - IF OTHER PARAMETERS THAT ARE REQUIRED ARE NOT GIVEN, ERRORS WILL RESULT.)

WASTE HEAT BOILER - EQUIPMENT TYPE 1.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	NUMBER OF BOILER TUBE PASSES	(1)	MS	MS	-
2.	BOILER TUBE LENGTH - ALL PASSES (FEET)	(2)	CM	MS	20.
3.	NUMBER OF TUBES - FIRST PASS	(2)	OE,CM	MS	-
4.	NUMBER OF TUBES - SECOND PASS	-	OE	MS	-
5.	NUMBER OF TUBES - THIRD PASS	-	OE	MS	-
6.	TUBE DIAMETER - FIRST PASS (INCHES)	(3)	OS	MS	-
7.	TUBE DIAMETER - SECOND PASS (INCHES)	(3)	OS	MS	-
8.	TUBE DIAMETER - THIRD PASS (INCHES)	(3)	OS	MS	-
9.	EXIT TEMPERATURE - FIRST PASS (DEG. F)	(4)	OS,CM	OE	1400.
10.	EXIT TEMPERATURE - SECOND PASS (DEG. F)	(4)	OS,CM	OE	900.
11.	EXIT TEMPERATURE - THIRD PASS (DEG. F)	(4)	OS,CM	OE	600.
12.	PRESSURE DROP (MAX.) - FIRST PASS (PSI)	(3)	OS	-	0.4
13.	PRESSURE DROP (MAX.) - SECOND PASS (PSI)	(3)	OS	-	0.4
14.	PRESSURE DROP (MAX.) - THIRD PASS (PSI)	(3)	OS	-	0.4
15.	COMBUSTION CHAMBER RESIDENCE TIME (SEC.)	(5)	CM	-	-
16.	MAX. RXN. HEAT RELEASE (BTU/HR.CU.FT.)	(5)	CM	-	-
17.	MUFFLE FURNACE LENGTH (FEET)	(6)	-	MS	-
18.	MUFFLE FURNACE DIAMETER (INCHES)	(6)	-	MS	-
19.	NO. 1 BYPASS RATIO (RANGE 0 - 1)	(7)	OE	MS	0.1
20.	NO. 1 BYPASS STREAM NUMBER	(8)	MS	MS	-
21.	NO. 2 BYPASS RATIO (RANGE 0 - 1)	(7)	OE	MS	0.1
22.	NO. 2 BYPASS STREAM NUMBER	(8)	MS	MS	-
23.	NO. 3 BYPASS RATIO (RANGE 0 - 1)	(7)	OE	MS	0.1
24.	NO. 3 BYPASS STREAM NUMBER	(8)	MS	MS	-
25.	BOILER EQUIL. CUTOFF TEMPERATURE (DEG. F)	(9)	OS	OS	1100.
26.	ADIABATIC FLAME TEMPERATURE (DEG. F)	-	OE	OE	2000.
27.	BOILER STEAM PRESSURE (PSIA)	-	OS	OS	250.
28.	BOILER TOTAL HEAT DUTY (BTU./HR.)	-	-	-	-

..... (CONTINUED)

NOTES - (WASTE HEAT BOILER)

1. - ONE, TWO OR THREE BOILER TUBE PASSES MAY BE USED.
2. - IF A MUFFLE FURNACE IS USED, THE BOILER TUBE LENGTH MUST BE GIVEN - IF A FIRE TUNNEL IS USED, THE NUMBER OF TUBES IN THE FIRST PASS MUST BE ONE.
3. - FOR EACH TUBE PASS, EITHER THE TUBE DIAMETER OR THE MAXIMUM ALLOWABLE TUBE PRESSURE DROP MAY BE GIVEN - IF NEITHER IS GIVEN, A PRESSURE DROP IS ASSUMED.
4. - ALL BOILER EXIT STREAM TEMPERATURES (INCLUDING BYPASS) MUST BE SPECIFIED FOR TUBE PASS DESIGN - INTERMEDIATE TUBE PASS TEMPERATURES MAY BE OPTIONALLY GIVEN.
5. - FOR COMBUSTION CHAMBER DESIGN (EITHER A FIRE TUNNEL OR A MUFFLE FURNACE), ONE OR BOTH OF RESIDENCE TIME AND MAXIMUM HEAT RELEASE MUST BE SPECIFIED.
6. - EFFECTIVE LENGTH AND DIAMETER MUST BE SPECIFIED FOR MUFFLE FURNACE SIMULATION.
7. - ALL BOILER BYPASS IS EXTRACTED FROM THE EXIT OF THE SECOND LAST PASS. BOILER BYPASS RATIOS MAY BE ESTIMATED FOR DESIGN - IF NOT, THE INDICATED VALUE IS USED AS AN INITIAL ESTIMATE. (SEE METHOD OF CALCULATING BOILER BYPASS STREAMS - APPENDIX A. AND ALSO NOTES ON INFORMATION FEED-BACK)
8. - 0.1, 0.2 OR 3 BYPASS STREAMS MAY BE USED. IF BYPASS STREAM EXISTS, THE STREAM NUMBER MUST BE SPECIFIED.
9. - THE ONLY REACTION ALLOWED BELOW THE EQUILIBRIUM CUTOFF TEMPERATURE IS THE SULPHUR SHIFT.

TABLE B-1 WASTE HEAT BOILER EQUIPMENT PARAMETERS

IN-LINE BURNER - EQUIPMENT TYPE 2.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	COMBUSTION CHAMBER EFFECTIVE LENGTH (FEET)	-	-	MS	-
2.	COMBUSTION CHAMBER DIAMETER (INCHES)	-	-	MS	-
3.	REACTION RESIDENCE TIME (SEC.)	(1)	CM	-	-
4.	MAX. RXN. HEAT RELEASE (BTU/HR.CU.FT.)	(1)	CM	-	-
5.	ADIABATIC FLAME TEMPERATURE (DEG. F)	(2)	OE	OE	2000.

NOTES -

1. - FOR COMBUSTION CHAMBER DESIGN, ONE OR BOTH OF COMBUSTION RESIDENCE TIME AND HEAT RELEASE MUST BE SPECIFIED.
2. - AS FOR THE BOILER, THE FLAME TEMPERATURE MAY BE ESTIMATED - IN LIEU OF A SPECIFIED ESTIMATE, THE INDICATED VALUE IS USED. IF A FLAME TEMPERATURE HAS BEEN FOUND PREVIOUSLY FOR EITHER AN IN-LINE BURNER OR FOR A BOILER COMBUSTION CHAMBER, THIS TEMPERATURE IS GIVEN THE HIGHEST PRIORITY AS AN ESTIMATE OF THE FLAME TEMPERATURE.

TABLE B-2 IN-LINE BURNER EQUIPMENT PARAMETERS

CONVERTER - EQUIPMENT TYPE 3.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	- CONVERTER NUMBER	-	OS	OS	-
2.	- CONV. BED CROSS-SECTIONAL AREA (SQ.FT.)	-	-	MS	-
3.	- CONVERTER BED DEPTH (FEET)	-	-	MS	-
4.	- CONVERTER BED VOLUME (CU.FT.)	-	-	-	-
5.	- PRESSURE DROP ACROSS THE BED (PSI)	-	-	-	-
6.	- MAX. SUPERFICIAL VELOCITY (FT./SEC.)	-	OS	-	1.0
7.	- MAX. MOLAL FLOWRATE (LB.MOLES/CU.FT.CAT)	(1)	OS	-	3.0
8.	- AVE. CATALYST PARTICLE DIAMETER (INCHES)	(2)	OS	OS	0.5

NOTES -

- 1. - THE VOLUME (REQUIRED BY THE SPECIFIED MOLAL FLOWRATE) DIVIDED BY THE CROSS-SECTIONAL AREA (REQUIRED BY THE SPECIFIED SUPERFICIAL VELOCITY) MAY RESULT IN A BED DEPTH LESS THAN 3 FEET. IN THIS CASE, 3 FEET IS USED AND A LOWER MOLAL FLOWRATE THAN SPECIFIED WILL RESULT.
- 2. - THE PARTICLE SIZE ONLY EFFECTS THE CALCULATED PRESSURE DROP CALCULATION. THUS, THE PARTICLE SIZE MAY BE ADJUSTED TO YEILD A REALISTIC PRESSURE DROP ACROSS THE BED.

TABLE B-3 CONVERTER EQUIPMENT PARAMETERS

CONDENSER - EQUIPMENT TYPE 4.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	- CONDENSER NUMBER	-	OS	OS	-
2.	- CONDENSER TUBE LENGTH (FEET)	-	-	MS	-
3.	- CONDENSER TUBE DIAMETER (INCHES)	-	OS	MS	1.0
4.	- NUMBER OF TUBES	-	-	MS	-
5.	- SHELL SIDE STEAM PRESSURE (PSIA)	-	OS	OS	50.
6.	- MAX. MASS VELOCITY (LB./SQ.FT.SEC.)	-	OS	-	4.0
7	- LIQUID SULPHUR STREAM NUMBER	-	MS	MS	-
8	- OUTLET GAS TEMPERATURE (DEG. F)	(1)	OS	-	-
9	- PERCENTAGE SULPHUR CONDENSATION	(1)	OS	-	95.
10.	- MAX. OUTLET FOG (LB. S./100 MOLES GAS)	-	OS	OS	-
11.	- ACTUAL SULPHUR RECOVERY (PERCENT)	(1)	-	-	-
12.	- CONDENSER HEAT LOAD (BTU./HR.)	-	-	-	-

NOTES -

1. - OUTLET CONDITIONS MAY BE SPECIFIED BY TEMPERATURE OR PERCENT CONDENSATION FOR THE LATTER CASE. THE TEMPERATURE (SATURATION) REQUIRED FOR THE DESIRED CONDENSATION IS FOUND. PERCENT CONDENSATION AND RECOVERY ARE NOT SYNONOMOUS - THE DIFFERENCE RESULTS FROM FOG FORMATION. OUTLET TEMPERATURE MAY BE SPECIFIED AS AN OUTLET STREAM SPECIFICATION.

TABLE B-4 CONDENSER EQUIPMENT PARAMETERS

ADIABATIC STREAM COMBINER - EQUIPMENT TYPE 5.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	- DESIRED COMBINER OUTLET TEMP. (DEG. F)	(1)	MS	-	425.
2.	- ACTUAL OUTLET TEMPERATURE (DEG. F)	-	-	-	-
3.	- STREAM NUMBER OF HOT STREAM INLET	(1)	MS	-	-

NOTES -

- FOR SIMULATION, NO SPECIFICATIONS ARE NECESSARY. FOR DESIGN, THE AMOUNT OF THE HOT STREAM REQUIRED TO HEAT THE (CORRESPONDINGLY REDUCED) COLD STREAM TO THE DESIRED OUTLET TEMPERATURE IS FOUND. A SULPHUR SHIFT IS DONE ON THE MIXED GASES, AND THE DESIRED STREAM IS USED AS THE COMBINER OUTLET STREAM. THIS CALCULATION IS DONE ONLY IF AN INFORMATION STREAM (RECYCLING A PRECEEDING STREAM SPLIT FRACTION) EXISTS - OTHERWISE THE STREAM OUTLET CONDITIONS RESULTING FROM THE GIVEN INLET STREAMS ARE USED. (SEE NOTES ON INFORMATION FEED-BACK)

TABLE B-5 ADIABATIC STREAM COMBINER EQUIPMENT PARAMETERS

STREAM COMBINER/DIVIDER - EQUIPMENT TYPE 6.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	- STREAM SPLIT FRACTION (RANGE 0 - 1)	(1)	OE	MS	0.1
2.	- OUTPUT STREAM FOR ABOVE SPLIT FRACTION	(1)	MS	MS	-

NOTES -

- FOR STREAM COMBINING (UP TO 5 STREAMS), NO SPECIFICATIONS ARE REQUIRED.
FOR SPLITTING THE INPUT STREAM(S) INTO TWO (2) OUTLET STREAMS, THE OUTLET
STREAM TO WHICH THE FEED TIMES THE SPLIT FRACTION IS TO BE DIRECTED MUST
BE GIVEN. (SEE INFORMATION FEED-BACK NOTES)

TABLE B-6 STREAM COMBINER/DIVIDER EQUIPMENT PARAMETERS

COMBUSTION AIR ADDER - EQUIPMENT TYPE 7.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	- STREAM NUMBER OF THE COMBUSTION AIR	(1)	MS	MS	-
2.	- RELATIVE HUMIDITY OF THE AIR (PERCENT)	-	OS	OS	50.
3.	- TEMPERATURE OF THE AIR (DEG. F)	(1)	OS	OS	70.
4.	- PRESSURE OF THE AIR (PSIA)	(1)	OS	OS	XX.
5.	- (DESIRED/STOICHIOMETRIC) AIR RATIO FOR H2S	(2)	OS	OS	1.0
6.	- (DESIRED/STOICHIOMETRIC) AIR RATIO FOR ALL	(3)	OS	OS	1.0

NOTES -

- 1. - A DUMY AIR STREAM MUST EXIST AND THE STREAM NUMBER GIVEN. AIR TEMP. AND PRESS. (BUT NOT REL. HUMID.) MAY BE GIVEN AS DUMY AIR STREAM PARAMETERS. IF THE AIR PRESSURE IS NOT SPECIFIED IN EITHER WAY, IT IS EQUATED TO THE ACID GAS PRESSURE.
- 2. - THIS RATIO DEFINES THE FRACTION OF THE INLET SULPHUR TO BE BURNED. IF THIS FRACTION IS NOT 1.0 (EG. 0.33333) THEN ALL INLET SULPHUR IS ASSUMED TO BE IN H2S FORM FOR COMBUSTION AIR CALCULATION PURPOSES.
- 3. - EXCESS OR DEFICIENT AIR FOR COMBUSTION OF SPECIFIED SULPHUR AND ALL CARBON AND HYDROGEN MAY BE SPECIFIED.

TABLE B-7 COMBUSTION AIR ADDER EQUIPMENT PARAMETERS

INCINERATOR - EQUIPMENT TYPE 8.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	- DESIRED INCINERATOR OUTLET TEMP. (DEG. F)	-	MS	-	-
2.	- COMBUSTION AIR REL. HUMIDITY (PERCENT)	-	OS	-	50.
3.	- COMBUSTION AIR TEMP. (DEG. F)	-	OS	-	70.
4.	- COMBUSTION AIR PRESSURE (PSIA)	(1)	OS	-	XX.
5.	- (DESIRED/STOICH.) AIR RATIO - PROCESS GAS	(2)	OS	-	1.25
6.	- (DESIRED/STOICH.) AIR RATIO - FUEL GAS	(2)	OS	-	1.25
7.	- STREAM NUMBER OF FUEL GAS	(3)	MS	MS	-

NOTES -

1. - IF NOT SPECIFIED, THE COMBUSTION AIR PRESSURE IS EQUATED TO THE TAIL GAS (INCINERATOR PROCESS INLET) PRESSURE.
2. - EXCESS (OR DEFICIENT) COMBUSTION AIR MAY BE ADDED TO THE PROCESS GAS AND/OR THE FUEL GAS.
3. - THE STREAM NUMBER OF THE FUEL GAS MUST ALWAYS BE GIVEN. FOR INCINERATOR DESIGN, THIS STREAM CONSISTS OF A STREAM TEMP. AND PRESS. AND A SAMPLE FUEL GAS COMPOSITION. NO AIR IS INCLUDED IN THIS CASE. FOR SIMULATION, THE FUEL GAS STREAM CONSISTS OF THE FUEL TO BE ADDED. IN THIS CASE, THE COMBUSTION AIR MAY BE ADDED WITH THE FUEL, OR MAY BE A SEPARATE INCINERATOR INLET STREAM (SPECIFIED).

TABLE B-8 TAIL GAS INCINERATOR EQUIPMENT PARAMETERS

STACK - EQUIPMENT TYPE 9.

P.N.	DESCRIPTION	NOTE	DES.	SIM.	VALUE
1.	- AMBIENT AIR TEMPERATURE (DEG. F)	-	OS	OS	70.
2.	- STACK OUTLET TEMPERATURE (DEG. F)	(1)	OS	OS	XX.
3.	- STACK HEIGHT (FEET)	-	-	MS	-
4.	- STACK DIAMETER (FEET AT TOP)	-	-	MS	-
5.	- MAX. GROUND CONCENTRATION (SO2,PPM)	-	OS	-	0.2
6.	- STACK VELOCITY (FT./SEC. AT TOP)	-	OS	-	60.
7.	- STACK VELOCITY INCREMENT (FT./SEC.)	(2)	OS	-	20.
8.	- NUMBER OF STACK VELOCITIES TO DO	(2)	OS	-	1.

NOTES -

- STACK OUTLET TEMPERATURE, IF NOT SPECIFIED, IS ASSUMED TO BE 200. DEG. F. LOWER THAN THE STACK INLET.
- A NUMBER OF STACKS WITH VARYING STACK VELOCITIES MAY BE DESIGNED. IN PRACTISE, VERY LITTLE DIFFERENCE IN REQUIRED STACK HEIGHT RESULTS (FOR A GIVEN MAX. GROUND CONC.) WITH VARYING STACK VELOCITY (STACK DIAMETER).

TABLE B-9 EFFLUENT STACK EQUIPMENT PARAMETERS

APPENDIX C

THIS APPENDIX CONTAINS PROGRAM DOCUMENTATION.

SUBROUTINE FUNCTIONS

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C.2 AUXILIARY ROUTINES C-4

C.3 COMPOSITION CALCULATION ROUTINES C-6

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FIG. C-2 SUBROUTINE LINKAGES C-25

TABLE C-1 PROGRAM CORE REQUIREMENTS C-26

C.1 EXECUTIVE AND UTILITY ROUTINES

ROUTINE -----	FUNCTIONS -----
MAIN -----	<ul style="list-style-type: none"> - MAINLINE EXECUTIVE ROUTINE - TRANSFERS CONTROL TO INPUT EXECUTIVE AND CALCULATION OPTIMIZATION EXECUTIVE - INITIALIZES EQUIPMENT MODULE CALCULATIONS AND CALLS APPROPRIATE EQUIPMENT MODULE FOR THE CALCULATIONS FOR EACH EQUIPMENT UNIT IN THE FLOWSHEET - CALLS CALCULATION SUMMARY ROUTINE WHEN PROCESS CALCULATIONS COMPLETED
RCYCL -----	<ul style="list-style-type: none"> - CALCULATION RECYCLE CONTROL ROUTINE - DETECTS IF AND WHEN PROCESS CALCULATION RECYCLE IS REQUIRED - RECYCLES CALCULATIONS WHEN ALL PREVIOUSLY ASSUMED STREAMS HAVE BEEN CALCULATED - CHECKS FOR RECYCLE CALCULATION CONVERGENCE WHEN RECYCLE LOOP COMPLETED - CONTROLS THE ACTIVE POSITION IN THE CALCULATION SEQUENCE VECTOR
TIMER -----	<ul style="list-style-type: none"> - COMPUTING TIME MONITOR ROUTINE - OPTIONALLY ACTIVATED BY COMPILE TIME DATA FLAG - USES 360/67 OS SYSTEM TIMER ROUTINES (CS019A AND CS019B) - OUTPUTS TIME INTERVAL SINCE LAST CALL AND TOTAL COMPUTING TIME TO CALL
PRINT -----	<ul style="list-style-type: none"> - OUTPUT CONTROL ROUTINE - SETS OUTPUT PRIORITY FLAG FOR MODULE CALCULATIONS BEFORE CONTROL IS TRANSFERRED BY EXECUTIVE TO EQUIPMENT MODULE - IF 'PRINT SUPPRESS' OPTION IS USED, CALCULATION OUTPUT IS SUPPRESSED FOR THE FIRST PASS THROUGH RECYCLE LOOPS - CONTROLS INITIALIZATION OF PAGING FOR EACH MODULE'S OUTPUT
FDSTM -----	<ul style="list-style-type: none"> - EXECUTIVE UTILITY ROUTINE - FINDS STREAM INPUTS TO ACTIVE EQUIPMENT NUMBER AND STORES IN A VECTOR (NSIN) IN THE ORDER PROCESS, SERVICE, INFORMATION -- LATTER TWO FLAGGED NEGATIVE - FINDS STREAM OUTPUTS FROM ACTIVE EQUIPMENT NUMBER AND STORES IN A VECTOR (NSOUT) AS ABOVE

DSECT -----	<ul style="list-style-type: none"> - EXECUTIVE DEBUG OUTPUT ROUTINE - OPTIONALLY DUMPS INPUT AND OUTPUT STREAMS AND RELEVANT SECTION OF EQUIPMENT PARAMETER VECTOR FOR ACTIVE EQUIPMENT NUMBER - CALLED BEFORE AND AFTER EACH EQUIPMENT MODULE CALCULATION - OUTPUT RESULTS ONLY IF EXECUTIVE DEBUG FLAG (IDBUG(15)) IS 4 OR GREATER
OUTPT -----	<ul style="list-style-type: none"> - PROCESS CALCULATION SUMMARY OUTPUT ROUTINE - OUTPUTS SUMMARY RESULTS IF EXECUTIVE OUTPUT FLAG (IDBUG(15)) IS 1 OR GREATER - OUTPUTS 'OVER ALL PLANT MASS AND ENERGY BALANCES', 'EQUIPMENT PARAMETER SUMMARY' AND 'STREAM COMPOSITION AND PROPERTY SUMMARY' WHEN ALL PROCESS CALCULATIONS ARE COMPLETE
SUTIL -----	<ul style="list-style-type: none"> - STREAM STORAGE UTILITY ROUTINE - DEPENDING UPON A FLAG, STORES A STREAM IN STREAM MATRIX (STREM), RETRIEVES A STREAM FROM STREAM MATRIX, OR COMBINES ALL INPUT STREAMS (WITH OPTIONAL EXCLUSION OF ONE INPUT STREAM) TO ACTIVE EQUIPMENT NUMBER. IN LAST CASE, RESULTING TEMPERATURE AND PRESSURE ARE FOUND
PRNTS -----	<ul style="list-style-type: none"> - STREAM OUTPUT UTILITY ROUTINE - OUTPUT RESULTS ONLY IF PRESENT OUTPUT PRIORITY FLAG IS 1 OR GREATER - OUTPUTS EQUIPMENT PROCESS FEED (COMBINED), PRESENT ACTIVE STREAM (YCOMP), OR STREAM FROM STREAM MATRIX, DEPENDING UPON A FLAG - TEMPERATURE, PRESSURE, ENTHALPY AND MOLE NUMBERS OF STREAM CONSTITUTE OUTPUT
COMPR -----	<ul style="list-style-type: none"> - DATA COMPATIBILITY CHECK UTILITY ROUTINE - COMPARES A STREAM PARAMETER (PARAMETER NSPAR OF STREAM NSTRM) WITH AN EQUIPMENT PARAMETER (PARAMETER NEPAR OF ACTIVE EQUIPMENT NUMBER) - IF ONE IS ZERO, THE TWO VALUES ARE EQUATED TO THE NEGATIVE SPECIFICATION VALUE - IF TWO VALUES ARE DIFFERENT (AND NON-ZERO) AN ERROR MESSAGE RESULTS -- BOTH VALUES ARE EQUATED TO EQUIPMENT PARAMETER VALUE
SETVU -----	<ul style="list-style-type: none"> - DEFAULT VALUE UTILITY FUNCTION - CHECKS A TEST VALUE -- IF POSITIVE, FUNCTION IS SET TO TEST VALUE - IF TEST VALUE IS ZERO OR NEGATIVE, FUNCTION IS SET TO DEFAULT VALUE

C.2 AUXILIARY ROUTINES

ROUTINE -----	FUNCTIONS -----
HFCAL -----	<ul style="list-style-type: none"> - THERMODYNAMIC PROPERTY EVALUATION ROUTINE - FOR GIVEN STREAM MOLE NUMBERS AND TEMPERATURE, EVALUATES (DEPENDING UPON A FLAG)-- <ul style="list-style-type: none"> - TOTAL STREAM HEAT CAPACITY, OR - TOTAL STREAM ENTHALPY, OR - ONE MOLECULAR SPECIE'S FREE ENERGY FUNCTION
VPRES -----	<ul style="list-style-type: none"> - VAPOR PRESSURE CALCULATION ROUTINE - DEPENDING UPON A FLAG, CALCULATES WATER OR SULPHUR VAPOR PRESSURE AT A GIVEN TEMPERATURE (ALSO FIRST DERIVATIVE OF VAPOR PRESSURE W. R. T. TEMPERATURE)
DEWPT -----	<ul style="list-style-type: none"> - DEW POINT CALCULATION ROUTINE - DEPENDING UPON A FLAG, CALCULATES WATER OR SULPHUR DEW POINT (USING NEWTON'S METHOD) FOR GIVEN PRESSURE AND STREAM MOLE NUMBERS - REQUIRES AN INITIAL ESTIMATE OF DEW PT. TEMP.
FINDT -----	<ul style="list-style-type: none"> - TEMPERATURE CALCULATION ROUTINE - GIVEN STREAM MOLE NUMBERS AND A REFERENCE ENTHALPY, FINDS THE CORRESPONDING TEMPERATURE ASSUMING NO COMPOSITION CHANGES (NEWTON'S METHOD USED) - REQUIRES AN INITIAL ESTIMATE OF TEMPERATURE
TCALC -----	<ul style="list-style-type: none"> - ITERATIVE TEMPERATURE DETERMINATION ROUTINE - FOR A GIVEN FEED STREAM, FINDS ADIABATIC OR NON-ADIABATIC TEMPERATURE, DEPENDING ON A FLAG - TAKES INTO ACCOUNT COMPOSITION CHANGES WITH TEMPERATURE - FOR NON-ADIABATIC CASE (BOILER), HEAT LOSS IS EVALUATED USING MEAN STREAM PROPERTIES (ALSO PRESSURE DROP IS CALCULATED AND REDUCED PRESSURE IS USED FOR OUTLET COMPOSITION CALCULATION) - TCTOF (EQUIL. CUTOFF TEMP.) MUST BE PREVIOUSLY SET - RIGOR OF CALCULATIONS INITIALLY IS LOW, BUT IS INCREASED AS CONVERGENCE (USING SECANT METHOD) IS ACHIEVED - INITIAL POSITIVE SET IS GENERATED FOR FIRST TEMPERATURE ESTIMATES, BUT THIS GENERATION IS BYPASSED WHEN CONVERGENCE IS NEARLY ACHIEVED - REQUIRES AN INITIAL ESTIMATE (TEMP)

- GUESR

- ESTIMATE GENERATOR ROUTINE
 - USES THE SECANT METHOD TO PREDICT THE INDEPENDENT VARIABLE THAT WILL RESULT IN A ZERO ERROR FUNCTION
 - GIVEN AN INITIAL ESTIMATE AND A FACTOR FOR GENERATING A SECOND ESTIMATE FROM THE FIRST, PRODUCES THIRD AND SUBSEQUENT ESTIMATES FROM PREVIOUS ERRORS AND ESTIMATES
 - SAVES BEST PREVIOUS ESTIMATE
 - MUST BE GIVEN A CONVERGENCE ACCELERATOR (USUALLY 1 IF NO CONVERGENCE PROBLEM) -- WILL EQUATE CONVERGENCE ACCELERATOR TO 1 AS CONVERGENCE PROCEEDS
- PROP

- STREAM PROPERTY EVALUATION ROUTINE
 - CALCULATES STREAM PROPERTIES USING AN AVERAGE STREAM COMPOSITION AND AVERAGE TEMPERATURE
 - EVALUATES AVERAGE COMPOSITION, AVERAGE AND WALL (SULPHUR DEW POINT) TEMPERATURES, GAS VISCOSITY, DENSITY, TOTAL STREAM MASS AND MOLES, AND AVERAGE STREAM HEAT CAPACITY
- SUMER

- STREAM SUMMER ROUTINE
 - DEPENDING UPON A FLAG, SUMS TOTAL MOLES AND MASS, TOTAL MOLES AND MASS OF ELEMENTAL SULPHUR OR, TOTAL ATOMS AND MASS OF (ATOMIC) SULPHUR IN A GIVEN STREAM
- PRCNT

- SULPHUR CONVERSION AND RECOVERY ROUTINE
 - CALCULATION BY-PASSED IF OUTPUT PRIORITY FLAG IS OFF
 - STORES INPUT SULPHUR, FINDS REAL AND APPARENT SULPHUR CONVERSION OR, FINDS TOTAL PLANT SULPHUR RECOVERY, DEPENDING UPON A FLAG
 - FOR LAST CASE, ALSO COMPLETES PLANT MASS AND ENERGY BALANCES
- STEAM

- STEAM PRODUCTION CALCULATION ROUTINE
 - FINDS CORRECTED LATENT HEAT OF STEAM AND STEAM PRODUCTION (LBS, AND MOLES) FOR A GIVEN DUTY, FEEDWATER STREAM AND STEAM TEMPERATURE
 - STORES RELEVANT STEAM FEED AND PRODUCT STREAMS IF PRESENT
- AIRFD

- COMBUSTION AIR REQUIREMENT ROUTINE
 - FINDS AIR STREAM (NITROGEN, OXYGEN AND WATER) REQUIRED TO COMPLETE A SPECIFIED COMBUSTION
 - REQUIRES FRACTION OF SULPHUR TO BE BURNED, EXCESS OR DEFICIENT AIR COEFFICIENT AND AIR RELATIVE HUMIDITY, PRESSURE AND TEMPERATURE SPECIFICATIONS
 - STORES AIR STREAM SEPARATELY -- ALSO ADDS AIR

TO GIVEN STREAM TO BE COMBUSTED AND FINDS
RESULTING COMBINED TEMPERATURE

- BKBOX

- (BLACK BOX) DUMMY EQUIPMENT MODULE (ITYPE=10)
 - SOLE EQUIPMENT PARAMETER IS TCTOF (EQUILIBRIUM CUTOFF TEMPERATURE) -- ASSUMED AS -1 IF NOT GIVEN (I.E. SULPHUR SHIFT ON GIVEN STREAM)
 - ALTERS INLET TEMPERATURE AND PRESSURE TO THE OUTLET CONDITIONS (TEMPERATURE AND PRESSURE) SPECIFIED AS *STREAM SPECIFICATION* DATA. IF LATTER IS NOT GIVEN, OUTPUT EQUATED TO INPUT
 - IF OUTPUT CONDITIONS (T AND P) GIVEN, COMPLETES COMPOSITION CALCULATION (DEPENDING UPON TCTOF) AT SPECIFIED OUTPUT CONDITIONS AND STORES OUTPUT MOLE NUMBERS. ENTHALPY DIFFERENCE BETWEEN INPUT AND OUTPUT IS CALCULATED.

C.3 COMPOSITION CALCULATION ROUTINES

- | ROUTINE
----- | FUNCTIONS
----- |
|------------------|---|
| COMP
----- | <ul style="list-style-type: none"> - PRIMARY COMPOSITION CALCULATION ROUTINE - DECIDES WHETHER TO DO COMPLETE EQUILIBRIUM CALCULATION AT GIVEN TEMPERATURE, EQUILIBRIUM AT CUTOFF TEMPERATURE, SULPHUR SHIFT ON CUTOFF COMPOSITION OR SULPHUR SHIFT ON GIVEN COMPOSITION - STORES CUTOFF EQUILIBRIUM COMPOSITION SO THAT IT NEED BE CALCULATED ONLY ONCE |
| SHIFT
----- | <ul style="list-style-type: none"> - SULPHUR SHIFT ROUTINE - EXTRACTS SULPHUR VAPOR SPECIES (AND OPTIONALLY LIQUID SULPHUR) FROM GIVEN STREAM -- INTRODUCES THEM INTO A DUMMY STREAM - CALCULATES EQUILIBRIUM COMPOSITION FOR THIS DUMMY STREAM AT GIVEN TEMPERATURE AND EXISTING SULPHUR PARTIAL PRESSURE. - ITERATES ON COMPOSITION CALCULATION UNTIL SULPHUR PARTIAL PRESSURE CONVERGES - SKIPS CALCULATION IF NO SULPHUR IN GIVEN STREAM |
| MINFE
----- | <ul style="list-style-type: none"> - FREE ENERGY MINIMIZATION ROUTINE - INITIALIZES THE EQUILIBRIUM CALCULATIONS - FOR EACH ITERATION, SETS UP THE MATRIX FOR DETERMINING THE LAGRANGIAN MULTIPLIERS - CALCULATES THE PREDICTED MOLE NUMBER CORRECTIONS |

INIT -----	<ul style="list-style-type: none"> - EQUILIBRIUM INITIALIZATION ROUTINE - DEPENDING UPON A FLAG, GENERATES A POSITIVE SET OF MOLE NUMBERS OR SKIPS THIS GENERATION - CALCULATES THE ATOM TOTALS, AND FREE ENERGY FUNCTIONS, AND FLAGS ALL IMPOSSIBLE SPECIES SO THEY WILL BE IGNORED DURING THE MINIMIZATION
YMODY -----	<ul style="list-style-type: none"> - COMPOSITION MODIFICATION ROUTINE - PREVENTS NEGATIVE OR PREMATURELY ZERO MOLE NUMBERS DURING ENERGY MINIMIZATION - DEFINES NEW MOLE NUMBERS AND CHECKS FOR CONVERGENCE OF THE COMPOSITION CALCULATIONS - EQUATES SPECIES DRIVEN BELOW A SPECIFIED LEVEL (I.E. $1.E-10$) TO ZERO AND FLAGS THEM SO THEY WILL BE IGNORED (THIS SPEEDS CONVERGENCE)
GAUSS -----	<ul style="list-style-type: none"> - GAUSSIAN ELIMINATION ROUTINE - SOLVES THE GIVEN MATRIX EQUATION FOR THE LAGRANGIAN MULTIPLIERS - PARTIAL PIVOTTING IS USED TO REDUCE ROUND-OFF ERRORS DURING CALCULATIONS - SINGULARITY OF THE MATRIX RESULTS IN JOB TERMINATION
FAKER -----	<ul style="list-style-type: none"> - EQUILIBRIUM COMPOSITION MASK ROUTINE - IF 'NDUMY' IS NON-ZERO, TEMPORARILY SETS THE NUMBER OF GASEOUS MOLECULAR SPECIES TO NDUMY. (I.E. THE FIRST NDUMY SPECIES ARE NOT MASKED, AND THE LAST (NGMS-NDUMY) SPECIES ARE MASKED, OR IGNORED DURING THE COMPOSITION CALCULATION WHICH IMMEDIATELY FOLLOWS) - MASKING OCCURS ONLY IF BOILER OR CONVERTER COMPOSITIONS ARE BEING CALCULATED, AND ONLY IF THE TEMPERATURE (AT WHICH THE COMPOSITION IS TO BE CALCULATED) IS LOWER THAN THE SPECIFIED SECONDARY CUTOFF TEMPERATURE (TDUMY).

C.4 DATA INPUT ROUTINES

ROUTINE -----	FUNCTIONS -----
INPUT -----	<ul style="list-style-type: none"> - DATA INPUT EXECUTIVE ROUTINE - INITIALIZES DATA INPUT AND THEN READS ALL DATA USING 'FFINP' FREE FORMAT INPUT ROUTINE - FOR EACH DATA SEGMENT OF INPUT, TRANSFERS CONTROL TO APPROPRIATE INPUT SUBROUTINE-- THIS ROUTINE IS DETERMINED FROM DECODED DATA CONTROL MESSAGES

- IF ANY ERRORS ARE DETECTED DURING DATA INPUT, THE JOB IS ABORTED WHEN DATA INPUT IS COMPLETE

INPT0

- PROGRAM CONTROL PARAMETER DATA INPUT ROUTINE
- SETS OUTPUT PRIORITY VECTOR (IDBUG) AND CONVERGENCE CRITERIA (CRIT) TO GIVEN OR DEFAULT VALUES
- SETS 'PRINT SUPPRESS' AND 'NO OPTIMIZATION' FLAGS IF DESIRED
- ECHO CHECKS THIS DATA IF DESIRED (IDBUG(14)=4 OR GREATER)

INPT1

- MOLECULAR AND THERMODYNAMIC DATA INPUT ROUTINE
- INITIALIZES M AND T DATA -- SETS THE NUMBER OF ATOMS TYPES, AND THE ATOM SYMBOLS, WEIGHTS AND VOLUMES
- STORES THERMODYNAMIC DATA (NASA) CONSTANTS AND VISCOSITY COEFFICIENTS IF GIVEN -- IF VISCOSITY COEFFICIENTS ARE NOT GIVEN, SETS THEM TO DEFAULT VALUES
- DEFINES THE NUMBER OF GASEOUS MOLECULAR SPECIES (NGMS) AND THE TOTAL NUMBER OF SPECIES (NTOT)
- CHECKS VALIDITY OF MOLECULAR SPECIES FORMULAS AND GENERATES THE FORMULA MATRIX (FORMU)

INPT2

- MOLECULAR AND THERMODYNAMIC DATA ANALYSIS ROUTINE
- CALCULATES MOLECULAR WEIGHTS AND VOLUMES
- DEFINES WHICH SPECIES ARE RADIATING COMPONENTS (FOR HEAT LOSS CALCULATIONS) -- ASSUMES SPECIES WITH THREE OR MORE CONSTITUENT ATOMS ARE POLAR AND RADIATING
- IDENTIFIES AND STORES WATER VAPOR COMPONENT AND SULPHUR VAPOR AND LIQUID COMPONENTS
- ECHO CHECKS M AND T DATA IF DESIRED (IDBUG(14) = 3 OR GREATER)

INPT3

- EQUIPMENT PARAMETER SPECIFICATION AND ESTIMATION DATA INPUT ROUTINE
- INITIALIZES EQUIPMENT PARAMETER VECTOR 'EQUIP' ELEMENTS TO ZERO
- DEFINES EQUIPMENT NUMBERS AND CORRESPONDING TYPES -- ALLOCATES EQUIP VECTOR STORAGE REQUIRED FOR EACH NUMBER AND STORES LOCATION IN AN INDEX
- STORES EQUIPMENT NUMBERS IN CALCULATION SEQUENCE VECTOR AS ENCOUNTERED. (THIS VECTOR IS NORMALLY RE-ORDERED LATER DURING CALCULATION SEQUENCE OPTIMIZATION)
- STORES EQUIPMENT PARAMETER SPECIFICATIONS IN EQUIP AS NEGATIVE VALUES DURING SPECIFICATION PHASE-- EQUIP PARAMETER ESTIMATES AS POSITIVE

- VALUES DURING ESTIMATION PHASE
- ECHO CHECKS SPECIFICATIONS AND ESTIMATES IF DESIRED (IDBUG(14)=1 OR GREATER)
- INPT4

- STREAM SPECIFICATIONS AND ESTIMATES DATA INPUT ROUTINE
 - INITIALIZES STREAM MATRIX (STREM) ELEMENTS TO ZERO
 - STORES STREAM SPECIFICATIONS AS NEGATIVE VALUES IN STREM, STREAM ESTIMATES (DURING ESTIMATES INPUT) AS POSITIVE VALUES
 - ECHO CHECKS SPECIFICATIONS AND ESTIMATES (SEPARATE INPUT DATA SECTIONS) IF THIS IS DESIRED (IDBUG(14)=2 OR GREATER)
- INPT5

- FLOWSHEET DATA INPUT ROUTINE
 - INITIALIZES FLOWSHEET MATRIX (INFO) ELEMENTS TO ZERO
 - SETS STREAM UNKNOWN TO 1 IF NOT GIVEN
 - STORES FLOWSHEET DATA IN INFO AND ECHO CHECKS IF DESIRED (IDBUG(14)=2 OR GREATER)
- FFINP

- FREE FORMAT INPUT ROUTINE
 - READS DATA AS FORTRAN ALPHAMERIC INPUT AND ANALYSES RESULTING ALPHAMERIC VECTOR A COLUMN AT A TIME
 - STORES INTEGERS, REALS AND ALPHAMERICS IN APPROPRIATE INPUT VECTORS AS ENCOUNTERED.
 - IGNORES REMAINDER OF CARD IF C ENCOUNTERED (DATA COMMENT)
 - CODES DATA CONTROL MESSAGES (ENCLOSED IN ASTERISKS) FOR INPUT ANALYSIS CONTROL
 - FLAGS ERROR IF SYNTAX ERROR ENCOUNTERED
- SPECL

- FINAL INPUT DATA CHECKING ROUTINE
 - CALLED WHEN DATA INPUT IS FINISHED TO COMPLETE DATA CHECKING AND DATA STORAGE
 - IDENTIFIES ATOM TYPES (S O C H N) IN THAT ORDER IF PRESENT
 - REARRANGES STREAM DATA TO CORRESPOND WITH REARRANGED M AND T DATA (I.E. LIQUID SPECIES STORED LAST)
 - CHECKS VALIDITY OF INFORMATION STREAMS (INFORMATION DESTINATIONS)

C.5 CALCULATION SEQUENCE OPTIMIZATION ROUTINES

ROUTINE -----	FUNCTIONS -----
OPTIM -----	<ul style="list-style-type: none"> - CALCULATION SEQUENCE OPTIMIZATION EXECUTIVE - INITIALIZES 'INFO' MATRIX FOR OPTIMIZATION (MASKS PLANT FEEDS AND PRODUCTS AND SERVICE STREAMS) - REDUCES THE FLOWSHEET -- TERMINATES THE OPTIMIZATION IF THE FLOWSHEET HAS BEEN COMPLETELY REDUCED - OPTIMIZES THE ORDER OF CALCULATIONS - RESTORES THE 'INFO' MATRIX WHEN OPTIMIZATION IS COMPLETE
REDUC -----	<ul style="list-style-type: none"> - FLOWSHEET SIMPLIFICATION ROUTINE - ATTEMPTS TO REDUCE THE COMPLEXITY OF THE FLOWSHEET (AND OPTIMIZATION) IN TWO PHASES - STORES ELIMINATED EQUIPMENT IN FINAL SEQUENCE VECTOR (PHASE 1) OR SAVES LINKS (PHASE 2) SO FINAL SEQUENCE CAN BE OBTAINED FROM OPTIMIZED REDUCED SEQUENCE WHEN OPTIMIZATION IS COMPLETE
DELTA -----	<ul style="list-style-type: none"> - ASSOCIATION MATRIX UTILITY ROUTINE - GENERATES THE 'IDELT' OR ASSOCIATION MATRIX FOR A GIVEN CALCULATION SEQUENCE USING THE FLOWSHEET DATA IN 'INFO' MATRIX
EXCHN -----	<ul style="list-style-type: none"> - SEQUENCE MODIFICATION UTILITY ROUTINE - ALTERS THE CALCULATION SEQUENCE AND THE ASSOCIATION MATRIX 'IDELT' IN THE MANNER DETECTED AS BEING ADVANTAGEOUS BY DCHCK - ALTERATION IS DONE DIRECTLY FOR SEQUENCE EXCHANGE OR BY CALLING DELTA FOR SEQUENCE PROMOTION OR DEMOTION
DCHCK -----	<ul style="list-style-type: none"> - SEQUENCE CHANGE SEARCH ROUTINE - ATTEMPTS TO FIND THE MOST BENEFICIAL CHANGE THAT CAN BE MADE TO THE CALCULATION SEQUENCE TO REDUCE RECYCLE ASSUMPTIONS - PREVENTS ALTERNATING BETWEEN TWO SEQUENCES
FINSH -----	<ul style="list-style-type: none"> - OPTIMIZATION MONITOR ROUTINE - DECIDES IF THE SEARCH FOR THE OPTIMUM SEQUENCE SHOULD BE CONTINUED UNINTERRUPTED, RENEWED WITH A RANDOMIZED SEQUENCE, OR TERMINATED - STORES BEST SEQUENCE AS ENCOUNTERED - RANDOMIZES THE CALCULATION SEQUENCE IF THIS IS

REQUIRED -- REBUILDS ASSOCIATION MATRIX (VIA
DELTA)

- SEQNC

- REGENERATES A FULL CALCULATION SEQUENCE USING THE SIMPLIFIED SEQUENCE AND THE LINKS STORED BY REDUC
 - FINDS THE STREAMS WHICH MUST BE ASSUMED FOR THE COMPLETE CALCULATION SEQUENCE (FINAL CALCULATION SEQUENCE IF A BETTER SEQUENCE IS NOT ENCOUNTERED)

C.6 EQUIPMENT MODULES ROUTINES

ROUTINE -----	FUNCTIONS -----
RXWHB -----	<ul style="list-style-type: none"> - PRIMARY REACTION FURNACE--WASTE HEAT BOILER ROUTINE - INITIALIZES CALCULATIONS -- DESIGNS OR SIMULATES THE COMBUSTION CHAMBER, AND ONE, TWO OR THREE BOILER PASSES - CALCULATES ONE, TWO OR THREE BYPASS STREAMS IF THEY EXIST AND STORES THE MAIN BOILER EXIT STREAM - FINDS STEAM PRODUCTION AND SULPHUR CONVERSION
BINIT -----	<ul style="list-style-type: none"> - BOILER INITIALIZATION ROUTINE - INITIALIZES BOILER CALCULATIONS -- DEFINES BOILER FEED, EQUILIBRIUM CUTOFF TEMPERATURE, BYPASS AND EXIT STREAMS, STEAM STREAMS AND BOILER STEAM PRESSURE - CALCULATES BOILER STEAM TEMPERATURE, CHECKS DATA COMPATIBILITY AND FLAGS WHETHER A MUFFLE FURNACE OR A FIRE TUNNEL IS USED
DOPAS -----	<ul style="list-style-type: none"> - BOILER TUBE PASS CALCULATION ROUTINE - SIMULATES OR DESIGNS BOILER TUBE PASSES - SIMULATION -- SINGLE PASS NON-ADIABATIC TEMPERATURE CALCULATION - DESIGN -- SINGLE OR MULTIPLE PASSES -- ITERATIVE TUBE NUMBER DETERMINATION - CALCULATES PRESSURE DROP AND/OR TUBE DIAMETER FOR EACH PASS - CALCULATES BOILER HEAT LOAD (DUTY)
FLAGI -----	<ul style="list-style-type: none"> - IFLAG UTILITY ROUTINE - SETS THE FLAG IFLAG FOR THE PASS (1 FOR DIAMETER SPECIFIED, PRESSURE DROP TO BE CALCULATED, 2 FOR TUBE DIAMETER AND PRESSURE DROP TO BE CALCULATED) - SETS BOILER LENGTH

- FLAGJ

- JFLAG UTILITY ROUTINE
 - SETS THE FLAG JFLAG FOR THE TUBE PASS (1 FOR SIMULATION -- (TUBE NUMBER GIVEN, EXIT TEMPERATURE TO BE CALCULATED), 2 FOR DESIGN -- (EXIT TEMPERATURE GIVEN, TUBE NUMBER TO BE DETERMINED))
 - DEFINES ESTIMATE FOR EITHER EXIT TEMPERATURE OR TUBE NUMBER
 - FLAGS FOR MULTIPLE TUBE PASS DESIGN IF THIS IS TO BE DONE
- NCALC

- BOILER TUBE NUMBER DETERMINATION ROUTINE
 - CALCULATES COMPOSITION AT SPECIFIED TUBE PASS EXIT TEMPERATURE
 - CALCULATES HEAT LOSS FOR EACH ESTIMATED TUBE NUMBER -- ITERATES ON TUBE NUMBER UNTIL DESIRED HEAT LOSS IS ACHIEVED
 - FOR EACH ESTIMATE TUBE DIAMETER AND/OR PRESSURE DROP ARE CALCULATED
 - FOR MULTIPLE TUBE PASS DESIGN, CALCULATES TOTAL HEAT LOSS FOR TUBE PASSES INVOLVED, USING AVERAGED COMPOSITION AND ESTIMATED INTERMEDIATE TUBE PASS EXIT TEMPERATURES -- TUBE PASSES INVOLVED ARE ASSUMED IDENTICAL
- HLOSS

- BOILER TUBE PASS HEAT LOSS CALCULATION ROUTINE
 - CALCULATES TOTAL HEAT LOSS (CONVECTIVE AND RADIATIVE) FOR A SINGLE PASS
 - IGNORES RADIATION EFFECT IF AVERAGE STREAM TEMPERATURE IS LESS THAN 900 DEG. F
 - USES GIVEN FEED TEMPERATURE, AVERAGE TUBE PASS COMPOSITION AND EITHER SPECIFIED OR ESTIMATED TUBE EXIT TEMPERATURE FOR CALCULATION OF HEAT LOSS
 - CALCULATES EMISSIVITY AND ABSORPTIVITY OF GAS BY LINEAR INTERPOLATION
- PDROP

- BOILER TUBE PASS PRESSURE DROP CALCULATION ROUTINE
 - CALCULATES PRESSURE DROP IF TUBE DIAMETER SPECIFIED (IFLAG=1)
 - FINDS MINIMUM VALID TUBE DIAMETER (FOR GIVEN TUBE NUMBER) WHICH WILL RESULT IN LESS THAN SPECIFIED MAXIMUM ALLOWABLE PRESSURE DROP (IFLAG=2)
 - FOR (IFLAG=2), STOPS ALTERNATION BETWEEN TWO DIAMETERS IF ALTERNATING SHOULD OCCUR
- INLNB

- PRIMARY IN-LINE BURNER ROUTINE
 - INITIALIZES CALCULATIONS -- THEN DESIGNS OR SIMULATES AN IN-LINE BURNER

- DEFINES EQUIPMENT FEED AND PRODUCT STREAMS
- BRNXC

- BURNER REACTION CHAMBER UTILITY ROUTINE
 - DESIGNS OR SIMULATES A COMBUSTION CHAMBER (IN-LINE BURNER, BOILER MUFFLE FURNACE OR BOILER FIRE TUNNEL)
 - FINDS ADIABATIC FLAME TEMPERATURE OF REACTION
 - DESIGN CASE -- FINDS SUITABLE COMBUSTION CHAMBER LENGTH AND DIAMETER
 - SIMULATION CASE -- FINDS REACTION RESIDENCE TIME AND UNIT VOLUME HEAT RELEASE
- CNVTR

- PRIMARY SULPHUR CONVERTER ROUTINE
 - INITIALIZES CALCULATIONS -- DEFINES FEED AND DESIGNS OR SIMULATES CONVERTER BED
 - DOES ADIABATIC REACTION TEMPERATURE CALCULATION
 - CHECKS DEW POINTS WITHIN THE CONVERTER BED
 - DEFINES OUTLET STREAM
- CRBED

- CONVERTER BED UTILITY ROUTINE
 - CALCULATES TOTAL MASS, MOLES, AND GAS VOLUME
 - DESIGN -- DETERMINES REQUIRED CROSS-SECTIONAL AREA AND DEPTH OF BED
 - SIMULATION -- CALCULATES MOLAR FLOWRATE AND SUPERFICIAL VELOCITY THROUGH THE BED
 - BOTH CASES -- CALCULATES PRESSURE DROP ACROSS THE BED
- DEWCK

- SULPHUR DEW POINT CHECK ROUTINE
 - DIVIDES CONVERTER BED TEMPERATURE RISE INTO INTERVALS -- DOES SULPHUR SHIFT AND THEN CALCULATES DEW POINT AT EACH INTERVAL -- CHECKS THAT IT IS BELOW BED TEMPERATURE
 - ASSUMES THAT CONVERSION REACTION IS LINEAR WITH TEMPERATURE ACROSS THE REACTION ZONE OF THE BED
- CONDR

- PRIMARY SULPHUR CONDENSER ROUTINE
 - INITIALIZES CALCULATIONS -- DEFINES CONDENSER FEED AND CALCULATES TOTAL INLET SULPHUR
 - DEFINES GAS AND SULPHUR OUTLET STREAMS AND STEAM STREAMS IF PRESENT
 - CHECKS DATA COMPATIBILITY
 - 'INTEGRATES' DOWN THE CONDENSER
 - CALCULATES RESULTING OVERALL HEAT TRANSFER COEFFICIENT, STEAM PRODUCTION, AND OUTLET FOG IN GASEOUS CONDENSER OUTLET STREAM
 - STORES CONDENSER OUTLET STREAMS.
- CINIT

- CONDENSER INITIALIZATION ROUTINE
 - SETS STEAM PRESSURE AND CALCULATES STEAM TEMPERATURE

- IDENTIFIES S8 AND LIQUID SULPHUR SPECIES
- INITIALIZES SULPHUR CONDENSATE FILM STREAM
- SETS CONDENSER TUBE DIAMETER
- DESIGN CASE -- DEFINES CONDENSER GAS OUTLET TEMPERATURE
- SIMULATION CASE -- DEFINES CONDENSER LENGTH
- EITHER CASE -- DEFINES NUMBER OF TUBES AND 'INTEGRATION' TEMPERATURE INTERVAL

CINTG

- CONDENSER 'INTEGRATION' ROUTINE
- INTEGRATES DOWN THE CONDENSER TUBES BY BREAKING THE CONDENSER INTO SEGMENTS DEFINED BY TEMPERATURES
- FOR EACH SEGMENT OUTLET TEMPERATURE, CALCULATES SULPHUR VAPOR PRESSURE AND MOLES OF SULPHUR AT SATURATION -- FINDS MINIMUM SULPHUR CONDENSATION FOR SEGMENT TO PREVENT SUPER-SATURATION AT OUTLET
- CALCULATES SEGMENT LENGTH AND PRESSURE DROP -- DOES A SULPHUR SHIFT AT EACH SEGMENT OUTLET
- AT END OF CONDENSER (DEFINED BY TEMPERATURE FOR DESIGN OR LENGTH FOR SIMULATION) RATIOS PORTION OF LAST SEGMENT TO USE. (ASSUMES COMPOSITION, PRESSURE, TEMPERATURE AND HEAT LOSS ARE LINEAR WITH LENGTH OVER LAST SEGMENT)

CSECT

- CONDENSER SEGMENT UTILITY ROUTINE
- FINDS CONDENSER SECTION AREA, HEAT LOSS AND OUTLET GAS (INCLUDING FOG FORMED) AND SULPHUR FILM STREAMS
- CALCULATES AVERAGE SEGMENT PROPERTIES, INCREMENTAL PRESSURE DROP, MOLECULAR VOLUME, DIFFUSIVITY AND GAS-SIDE HEAT TRANSFER COEFFICIENT

CHBAL

- CONDENSATE FILM HEAT BALANCE ROUTINE
- ITERATIVELY ESTIMATES THE SEGMENT SULPHUR FILM TEMPERATURE SUCH THAT THE FILM HEAT BALANCE IS SATISFIED
- CALCULATES SULPHUR VAPOR PRESSURE AND LATENT HEAT OF VAPORIZATION AT FILM TEMPERATURE, MASS TRANSFER COEFFICIENT, HEAT LOSS FROM GAS TO FILM AND FROM FILM TO STEAM FOR EACH ESTIMATE OF FILM TEMPERATURE

AQFND

- CONDENSER SEGMENT HEAT BALANCE ROUTINE
- ITERATIVELY ESTIMATES THE SEGMENT LENGTH SUCH THAT A HEAT BALANCE ON THE SEGMENT IS SATISFIED
- FOR EACH ESTIMATE OF LENGTH, THE SEGMENT MASS AND HEAT TRANSFER ARE CALCULATED -- THE SEGMENT OUTLET STREAMS ARE FOUND AND THEIR ENTHALPY IS CALCULATED
- CHANGE IN SEGMENT STREAM ENTHALPIES MUST

EQUAL SEGMENT HEAT LOSS

- SEGMENT OUTLET MUST BE SATURATED OR SUPER-HEATED
- OTHERWISE FOG IS FORMED UNTIL SATURATION IS REACHED

FOGST

- CONDENSER OUTLET FOG DETERMINATION ROUTINE
- SETS OUTLET FOG TO SPECIFIED MAXIMUM IF THIS HAS BEEN SPECIFIED
- CALCULATES CONDENSER PERCENTAGE CONDENSATION AND SULPHUR RECOVERY
- STORES CONDENSER OUTLET STREAMS

COMBN

- PRIMARY ADIABATIC STREAM COMBINER ROUTINE
- DEFINES EQUIPMENT FEED
- CHECKS DATA FOR COMPATIBILITY
- FINDS ADIABATIC OUTLET TEMPERATURE (SULPHUR SHIFT REACTION ALLOWED ONLY)
- IF INFORMATION RECYCLE STREAM EXISTS, PREDICTS WHAT UPSTREAM STREAM SPLIT SHOULD BE TO YIELD DESIRED OUTLET TEMPERATURE. (USES RESULTS OF THIS PREDICTION AS PRESENT EQUIPMENT OUTLET STREAM)
- CALCULATES OUTLET STREAM SULPHUR AND WATER DEW POINTS AND STORES RESULTING OUTLET STREAM

FINDE

- STREAM SPLIT PREDICTOR ROUTINE
- DEFINES INFORMATION STREAM AND HOT AND COLD PROCESS INLET STREAMS
- USING THE SECANT METHOD, ITERATIVELY ESTIMATES UPSTREAM SPLIT TO YIELD DESIRED OUTLET TEMPERATURE
- FOR EACH ESTIMATE, EVALUATES EFFECTS ON HOT AND COLD STREAMS -- DOES SULPHUR SHIFT AND THEN FINDS RESULTING OUTLET TEMPERATURE (NEWTON'S METHOD)
- STORES PREDICTED SPLIT IN INFORMATION STREAM WHEN CONVERGENCE ACHIEVED

CMBDV

- PRIMARY STREAM COMBINER/DIVIDER ROUTINE
- COMBINES UP TO 5 INLET STREAMS AND CALCULATES RESULTING TEMPERATURE AND PRESSURE
- DIRECTS COMBINED STREAMS TO A SINGLE OUTPUT OR DIVIDES THE STREAM BETWEEN TWO OUTLETS

AIRAD

- PRIMARY COMBUSTION AIR ADDER ROUTINE
- DEFINES ACID GAS FEED AND IDENTIFIES AIR STREAM
- FINDS AIR REQUIREMENTS AND ADDS AIR TO ACID GAS TO FORM OUTPUT STREAM
- STORES OUTPUT AND AIR INLET STREAMS

INCIN

- PRIMARY TAIL GAS INCINERATOR ROUTINE
- IDENTIFIES FUEL GAS STREAM AND DEFINES FEED

- VAPORIZES ANY INLET LIQUID SULPHUR
- SIMULATION -- COMBINES PROCESS GAS INLET AND (FUEL AND AIR) INLET AND DETERMINES THE ADIABATIC FLAME TEMPERATURE
- DESIGN -- ITERATIVELY ESTIMATES THE AMOUNT OF FUEL (AND AIR) REQUIRED TO ACHIEVE THE DESIRED OUTLET TEMPERATURE. FOR EACH ESTIMATED FUEL AND AIR ADDITION, CALCULATES RESULTING TEMP.
- CONVERGENCE ACHIEVED USING SECANT METHOD
- STORES OUTLET STREAM (AND AIR AND FUEL STREAM FOR THE DESIGN CASE)

STACK -----

- PRIMARY EXHAUST GAS STACK ROUTINE
- IDENTIFIES SO₂ (POLLUTANT SPECIE)
- CALCULATES EQUIVALENT AMBIENT AND STACK OUTLET TEMPERATURES, TOTAL AND POLLUTANT FLOWRATES AND STACK VELOCITY
- DETERMINES REQUIRED STACK HEIGHT (DESIGN) OR MAX GROUND CONCENTRATION OF POLLUTANT (SIMULATION)
- OPTIONALLY DESIGNS SEVERAL STACKS WITH VARYING STACK VELOCITIES

STAKU -----

- STACK UTILITY ROUTINE
- CALCULATES MAXIMUM GROUND CONCENTRATION OF POLLUTANT (SO₂) AND DISTANCE TO THE MAXIMUM AT SEVERAL WIND VELOCITIES FOR BOTH MODERATELY STABLE AND MODERATELY UNSTABLE ATMOSPHERIC CONDITIONS
- THE MINIMUM STACK HEIGHT REQUIRED FOR A MAXIMUM ALLOWABLE GROUND CONCENTRATION IS FOUND IN THE DESIGN CASE.
- FOR THE SIMULATION CASE, THE MAXIMUM GROUND CONCENTRATION, THE CORRESPONDING WIND SPEED AND DISTANCE TO THE MAXIMUM FOR A GIVEN STACK HEIGHT ARE FOUND

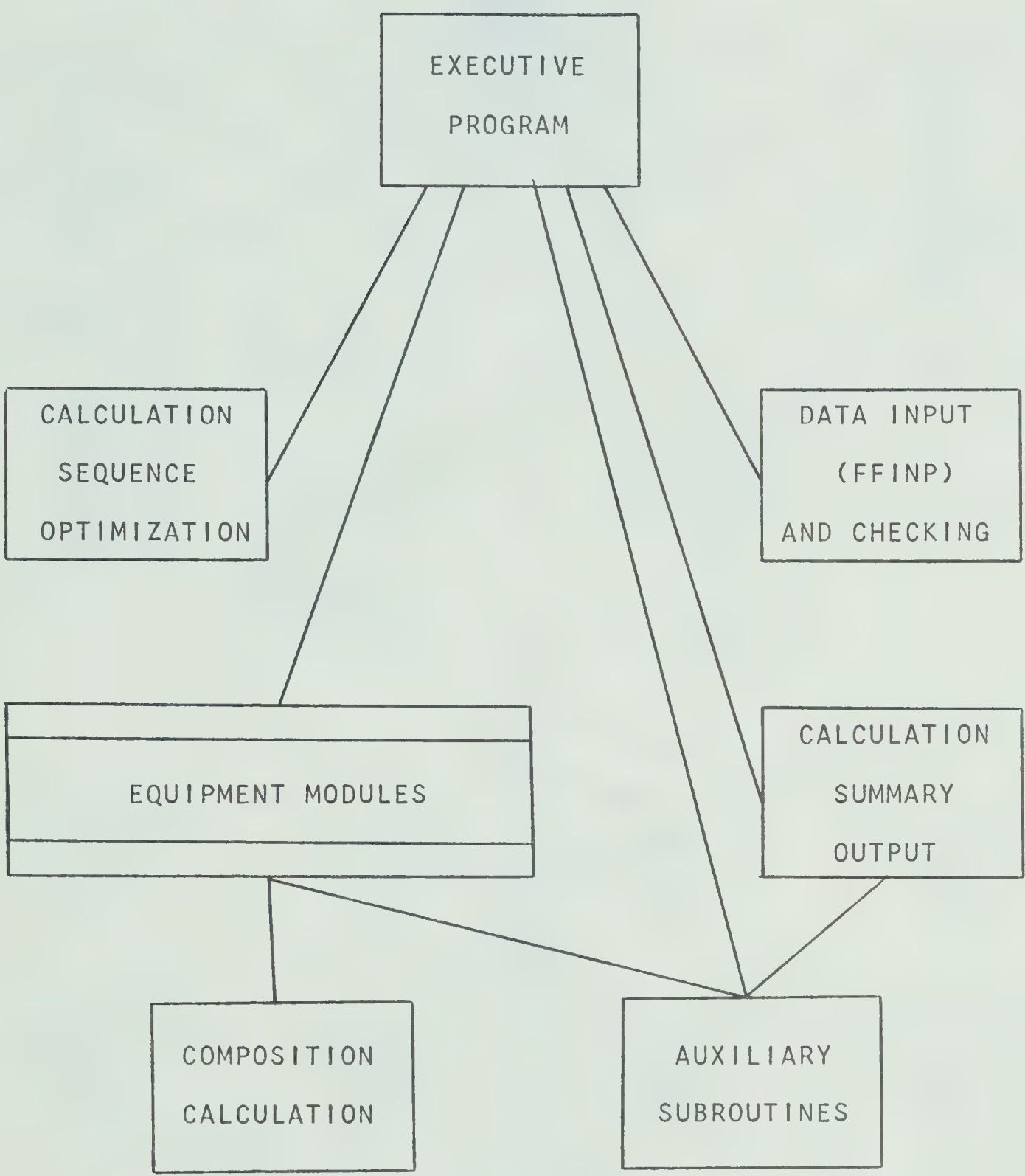
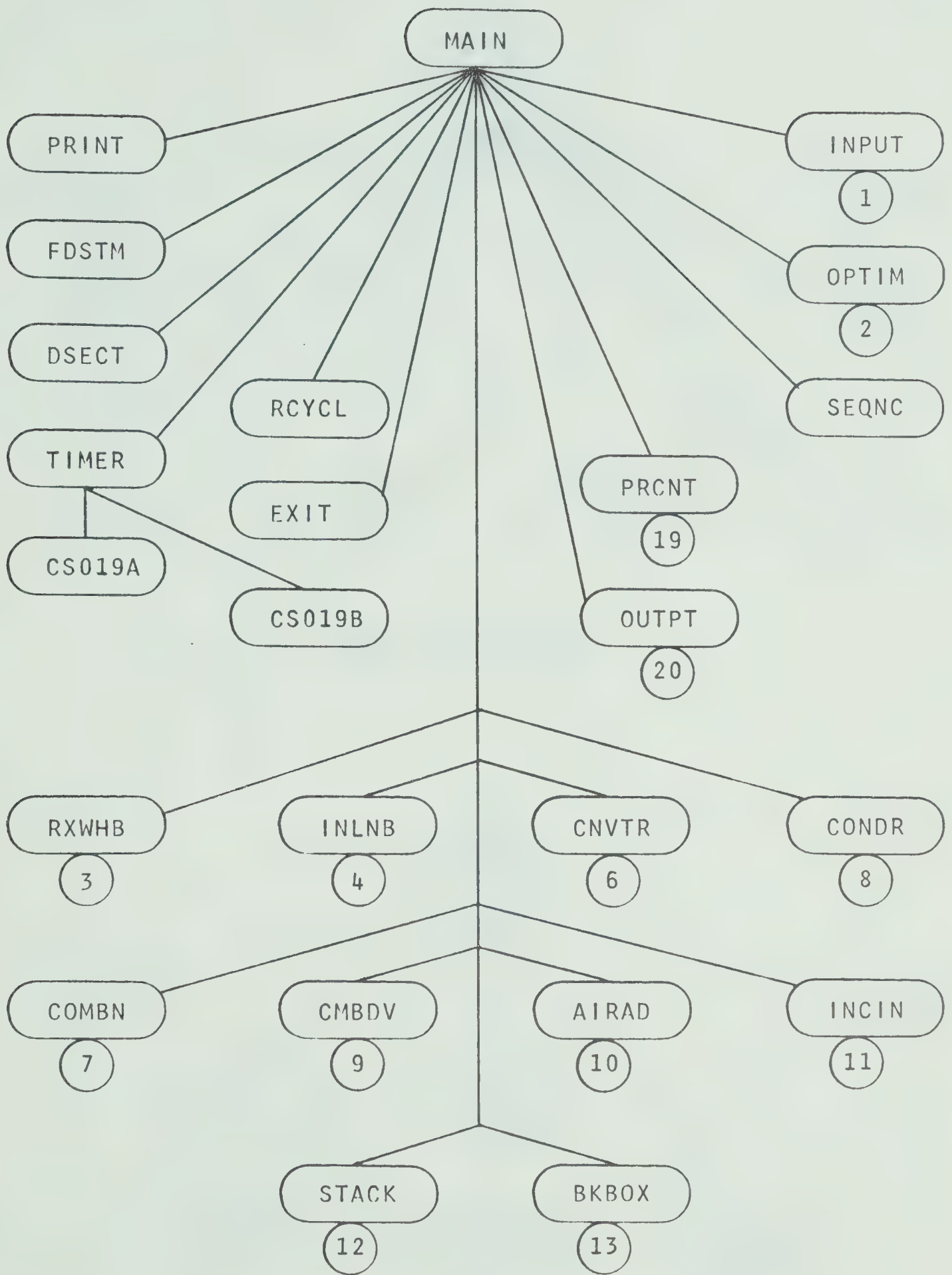
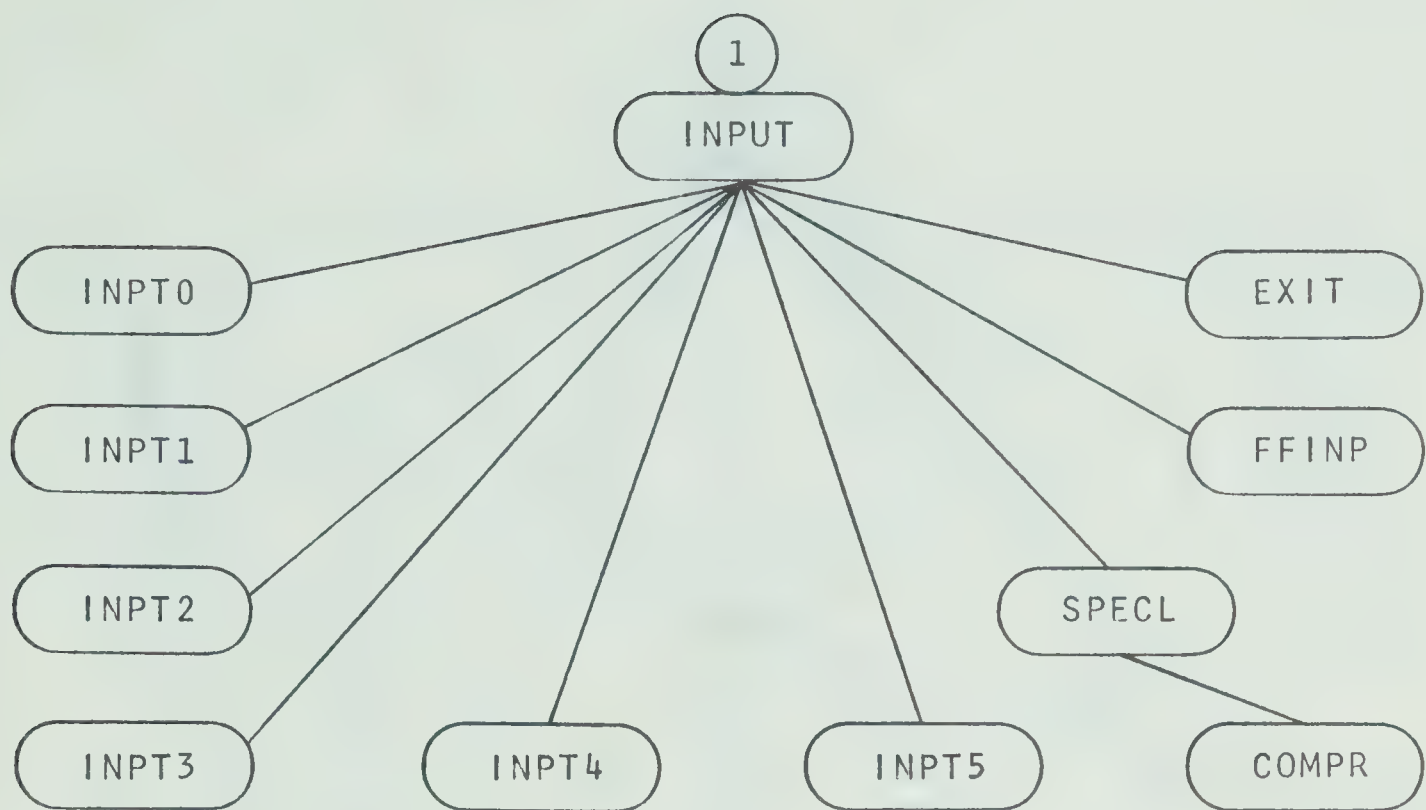


FIG. C-1 PROGRAM STRUCTURE

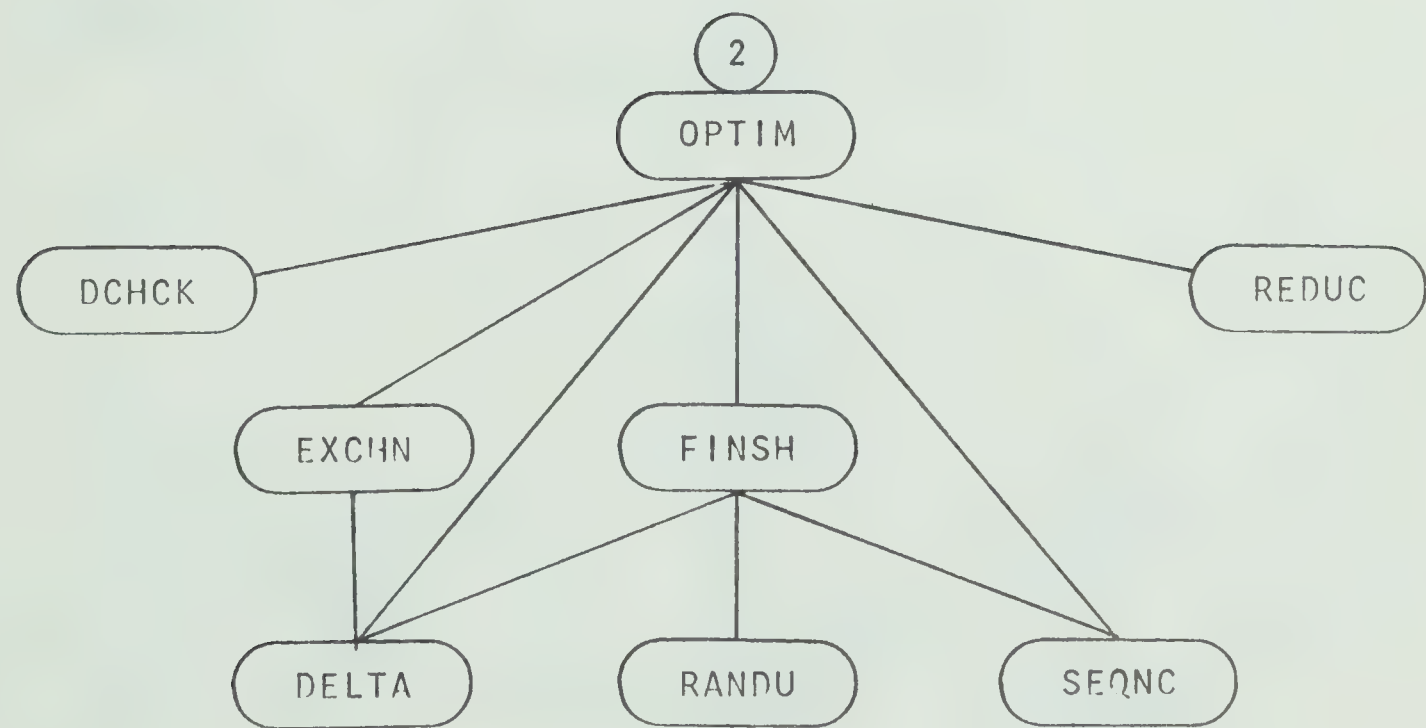


MAINLINE EXECUTIVE

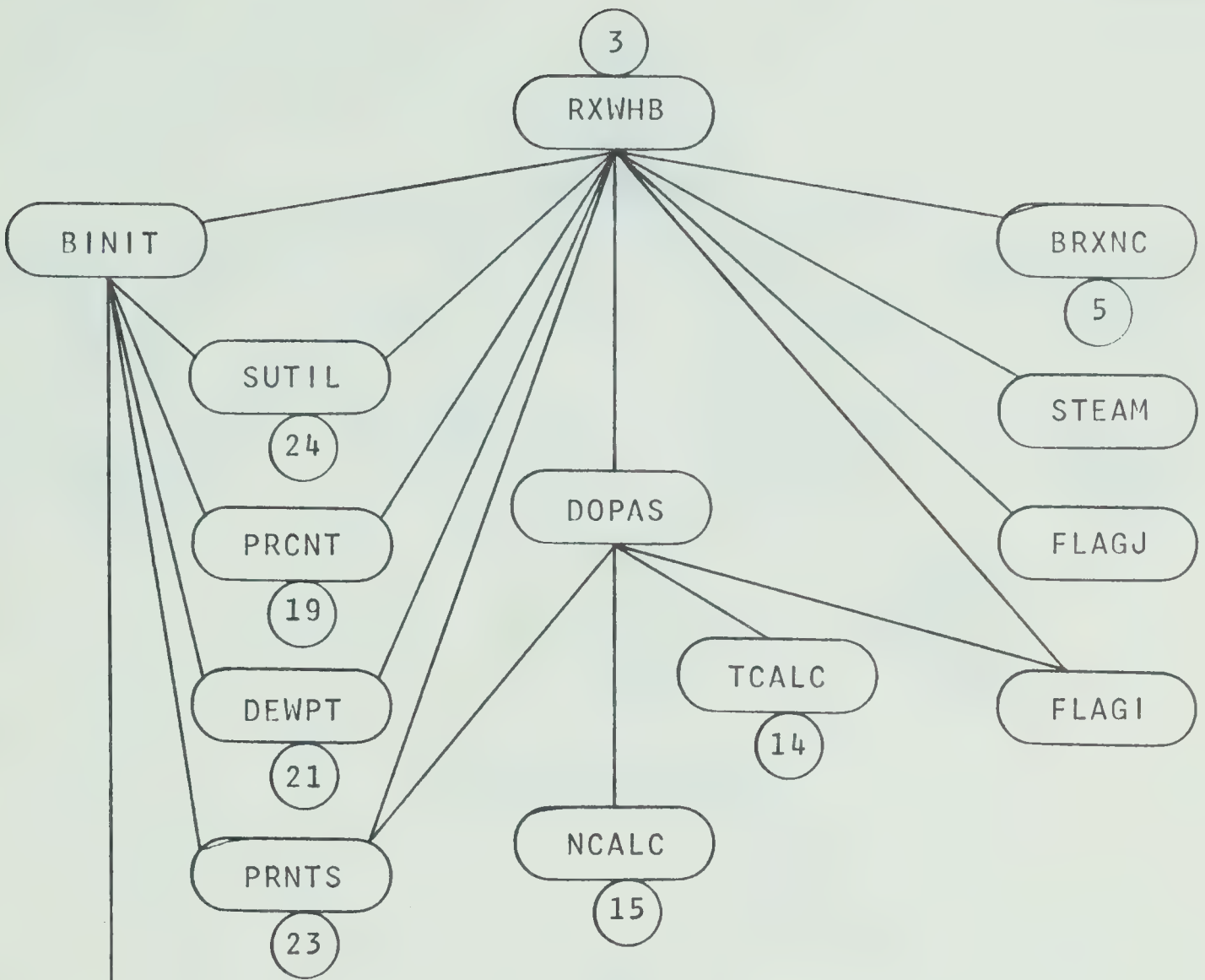
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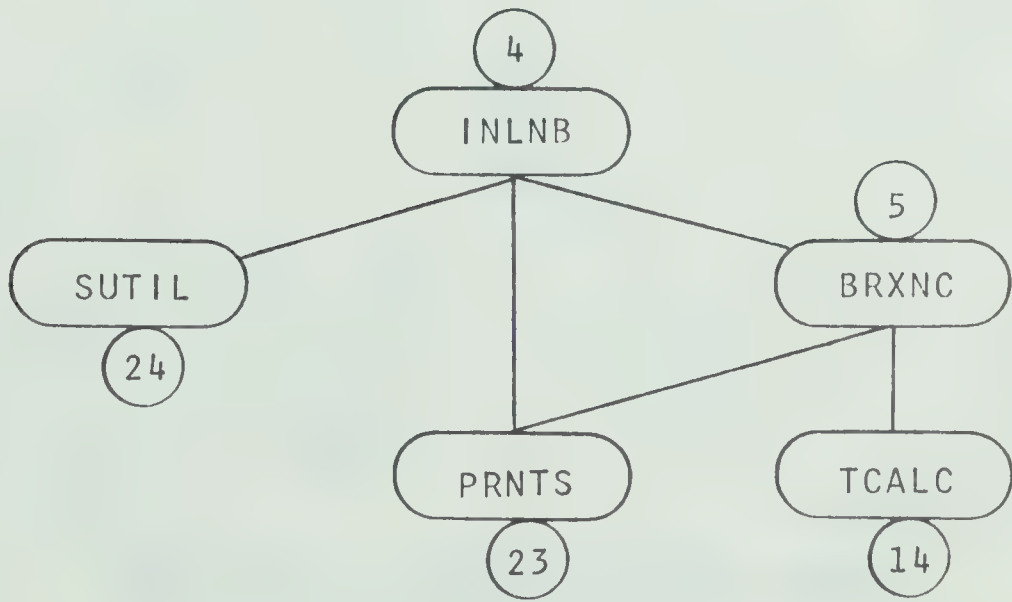
DATA INPUT MODULE



CALCULATION SEQUENCE OPTIMIZATION MODULE

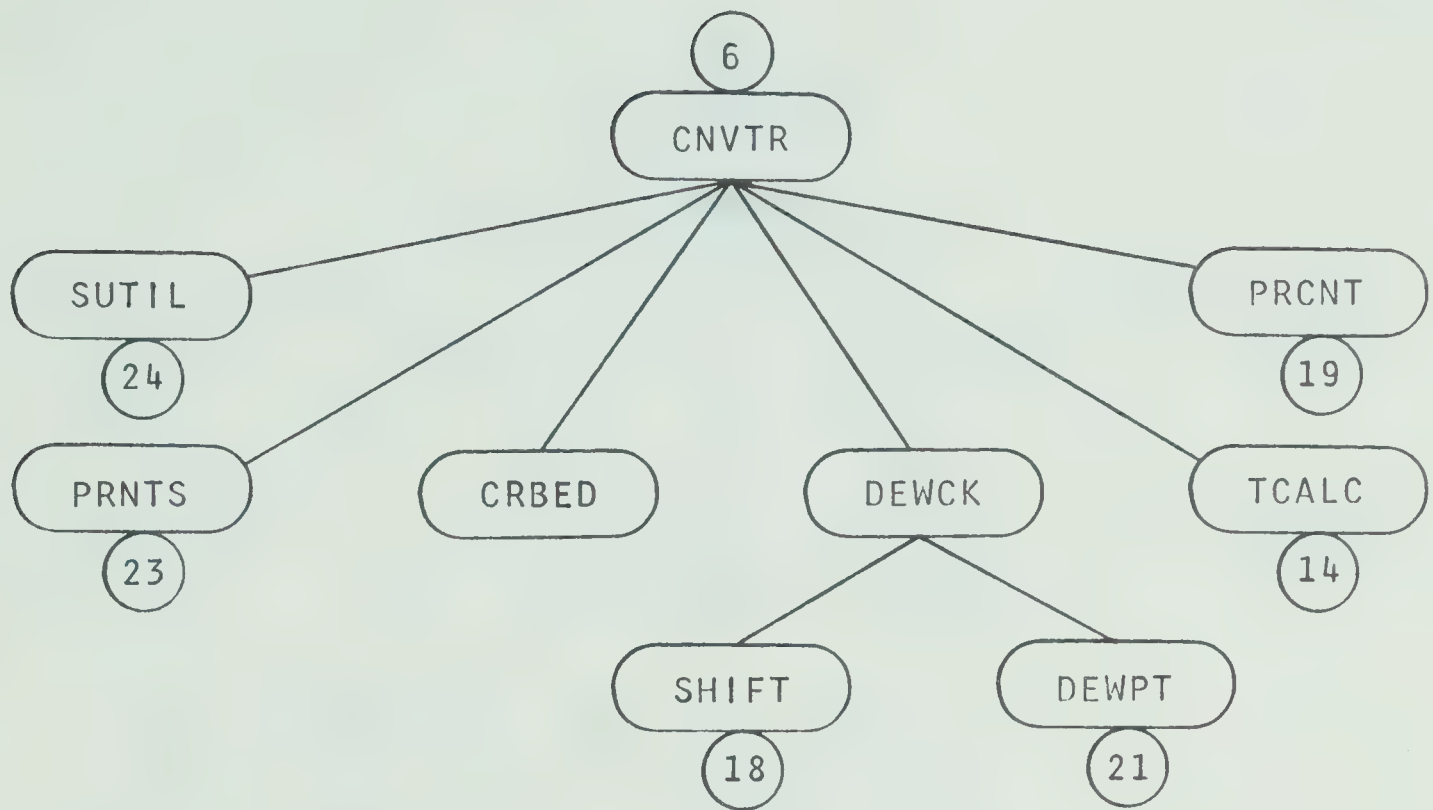


WASTE-HEAT BOILER MODULE

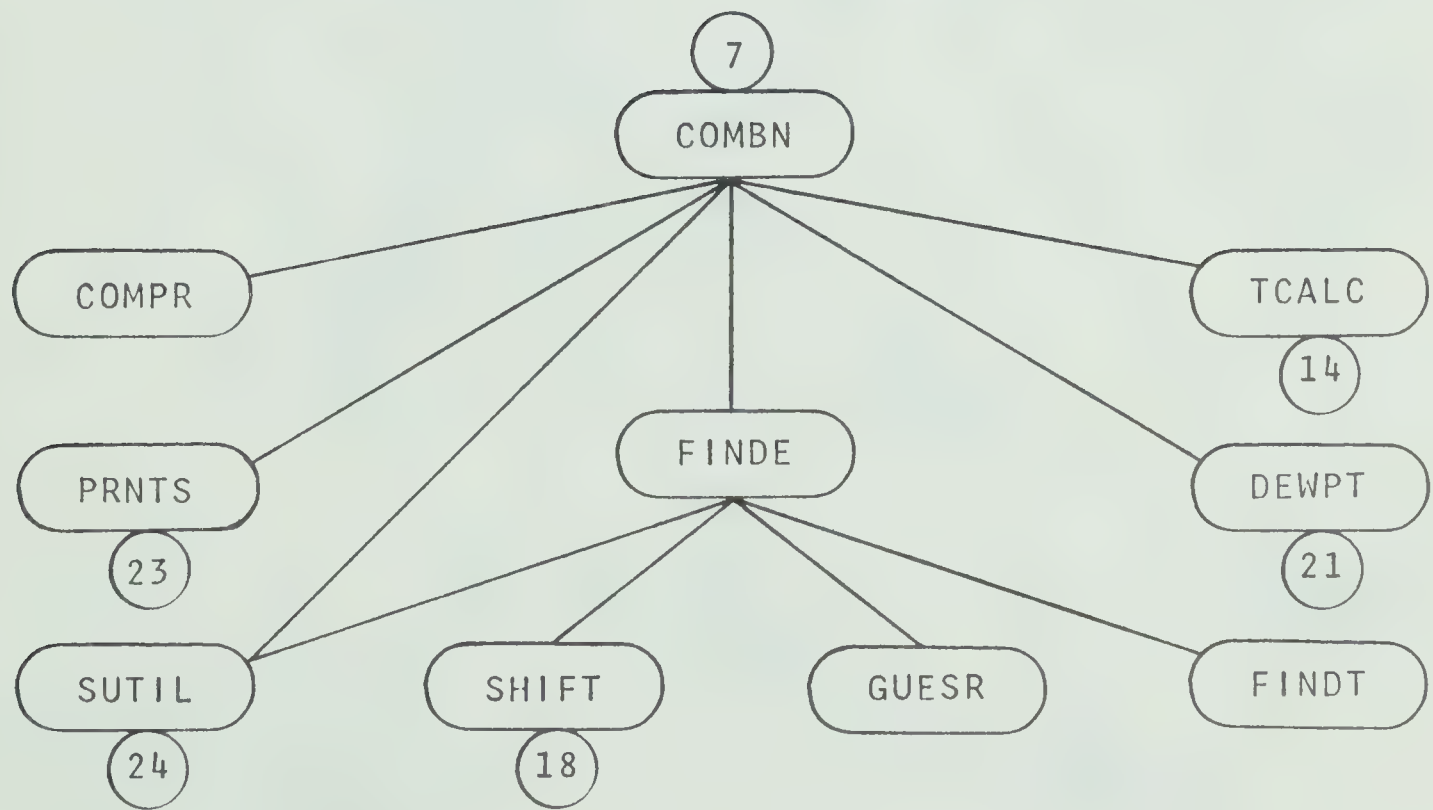


INLINE BURNER MODULE

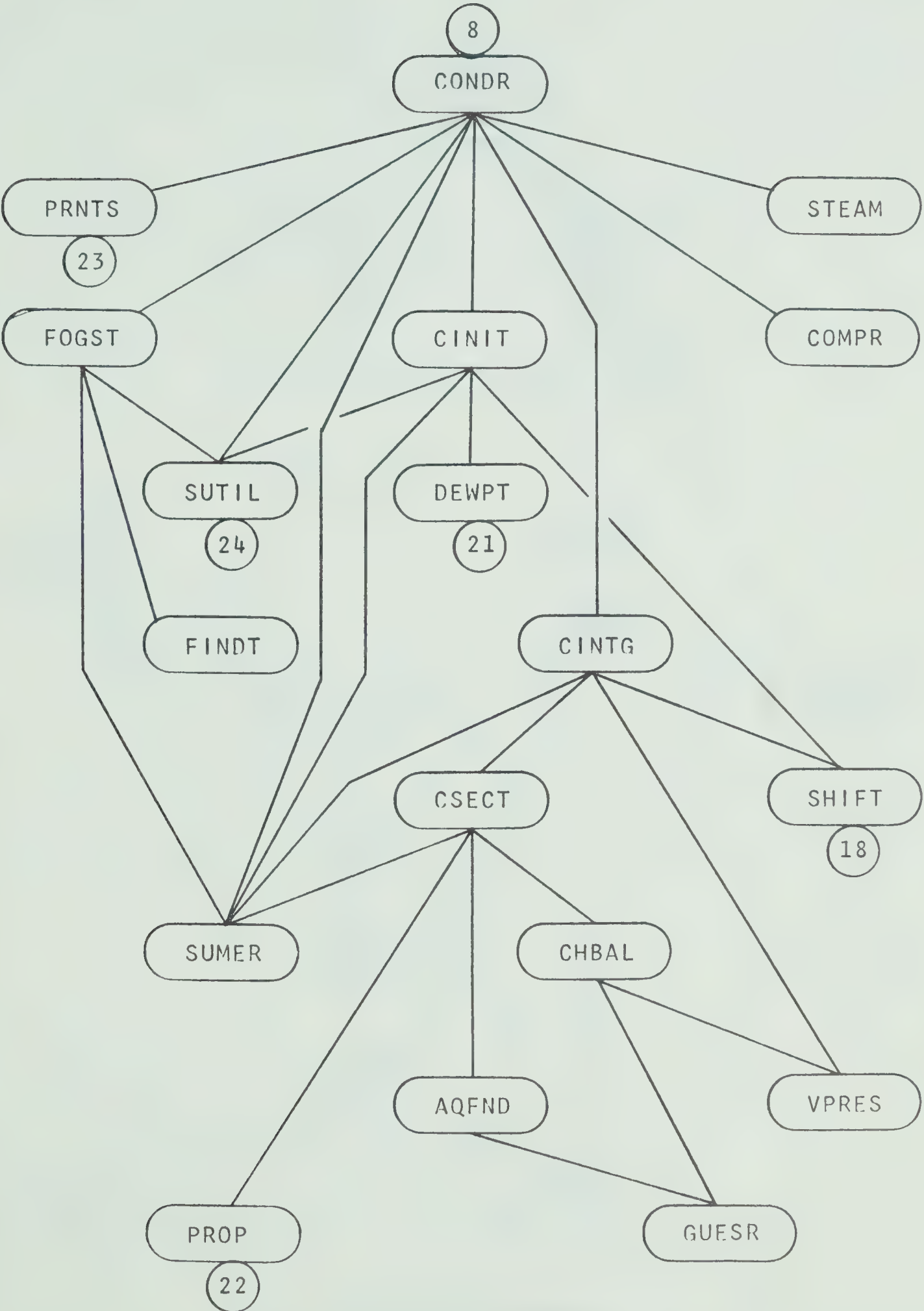
.... continued



CONVERTER MODULE

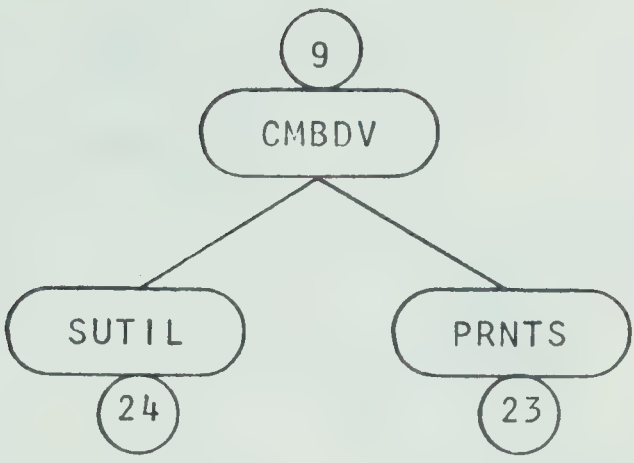


ADIABATIC STREAM COMBINER MODULE

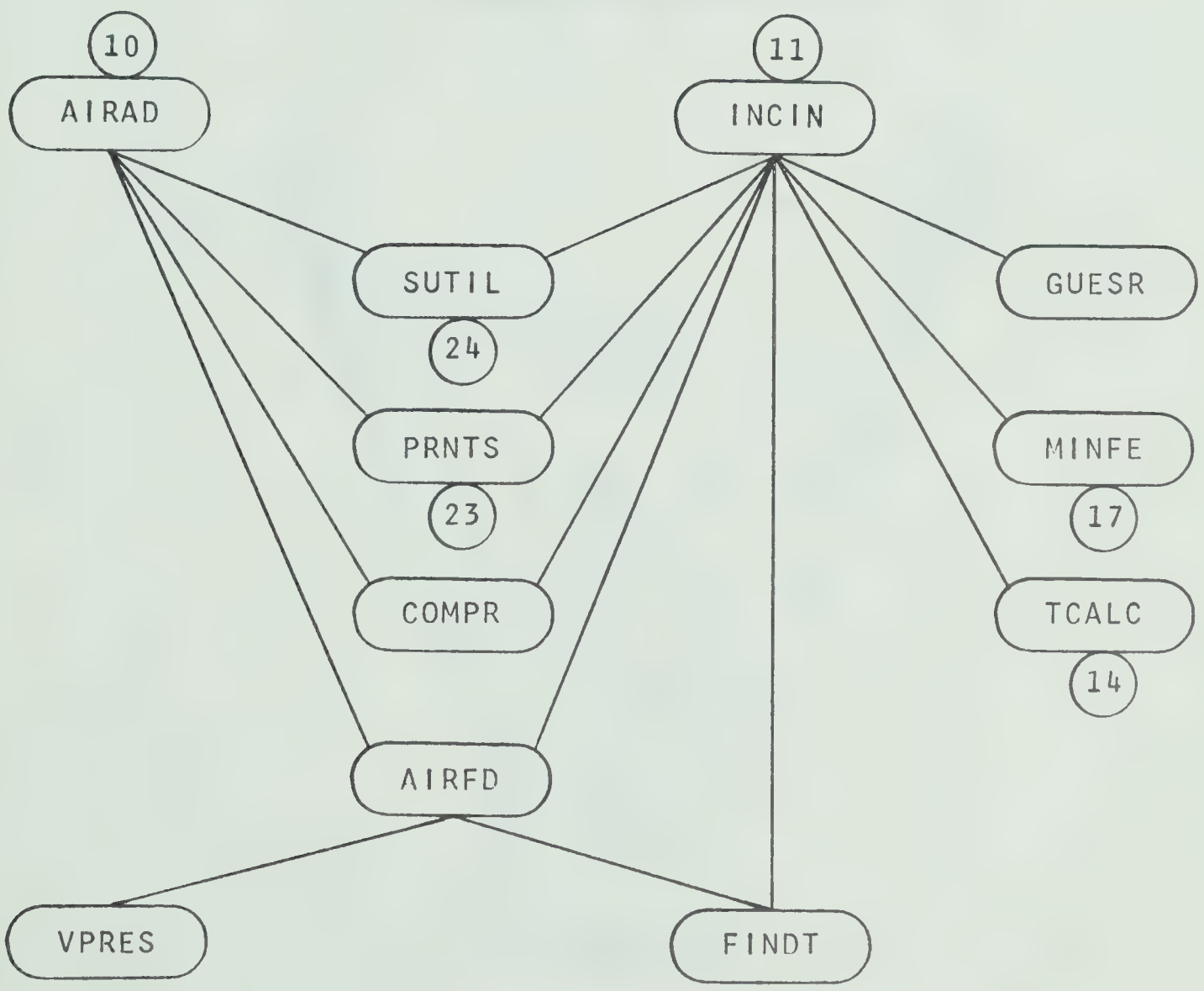


CONDENSER MODULE

.... continued

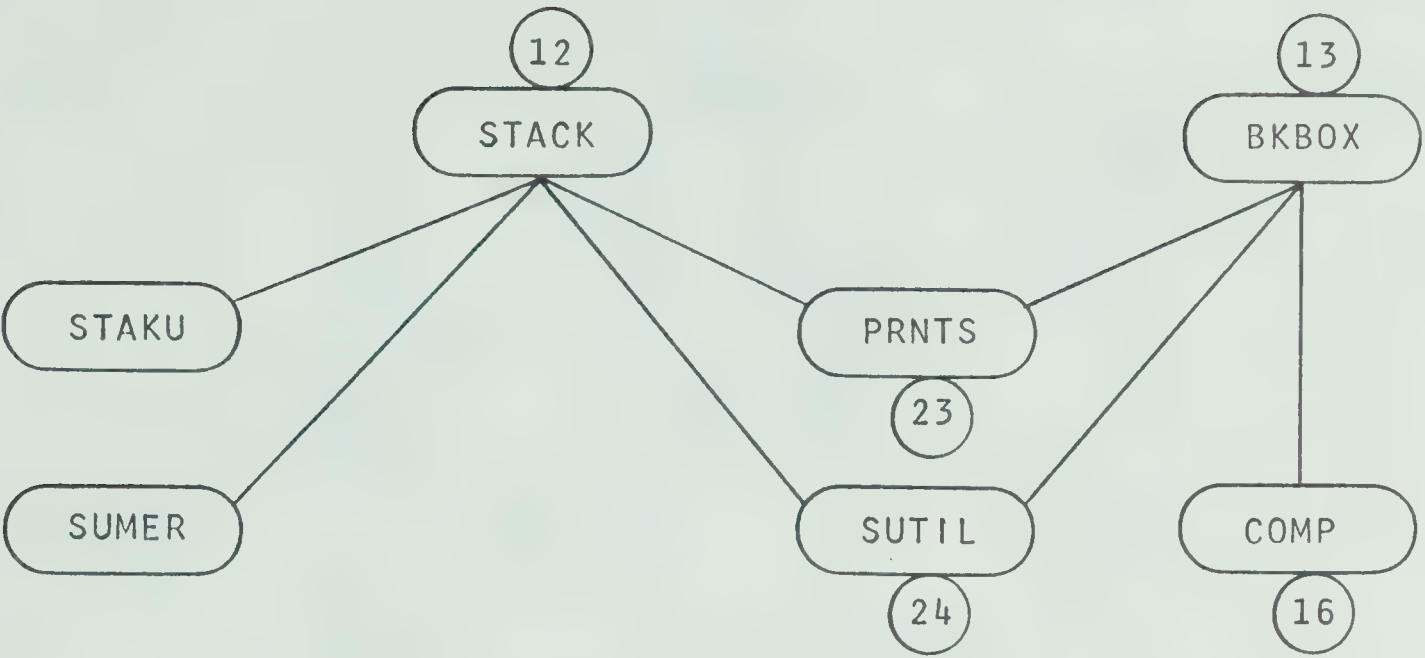


STREAM COMBINER/DIVIDER MODULE

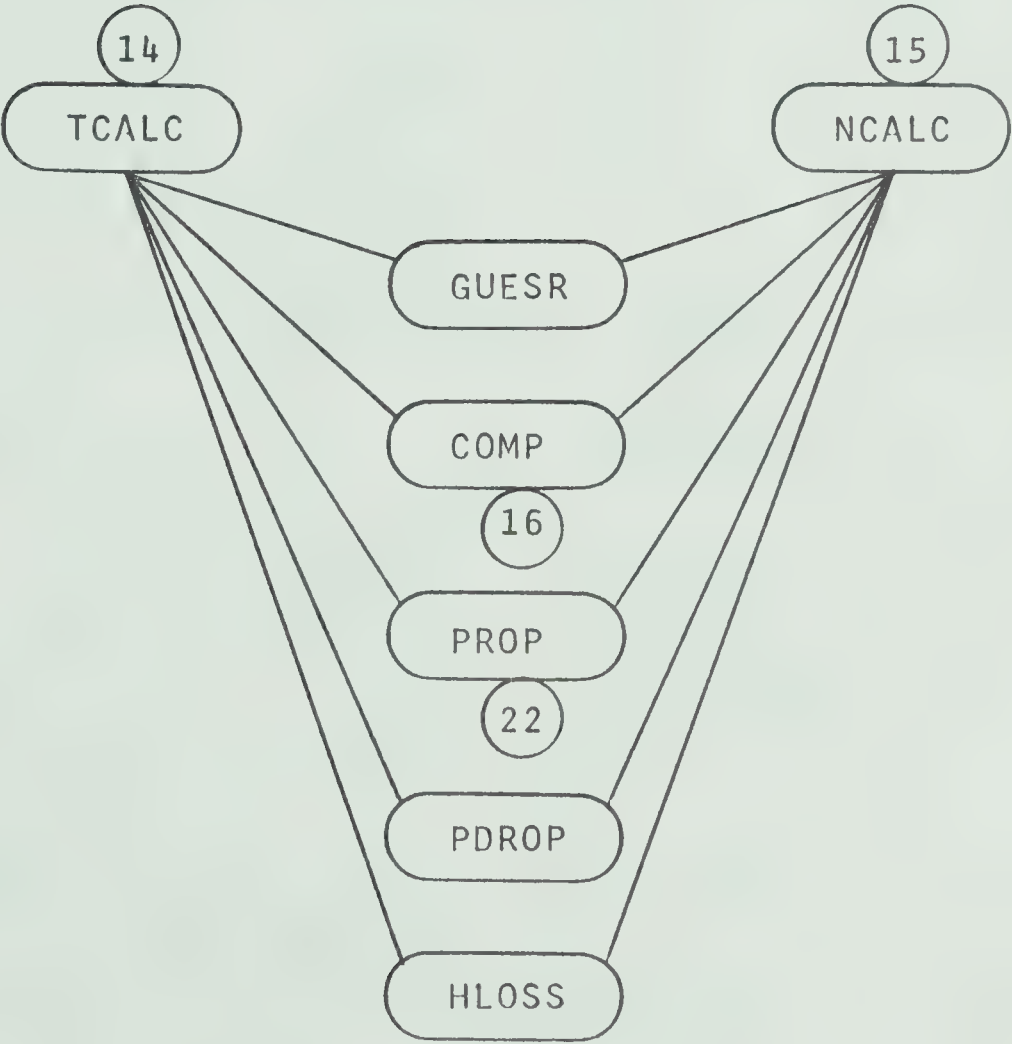


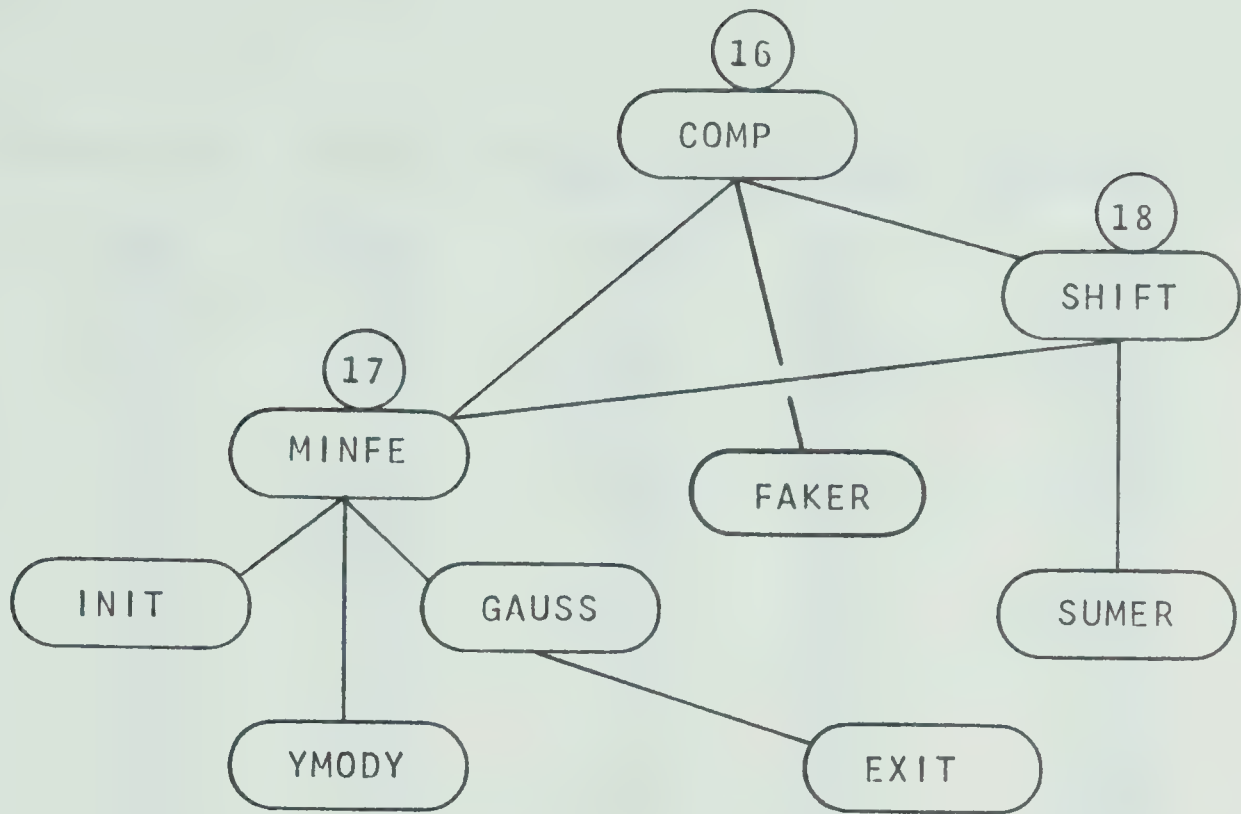
INCINERATOR MODULE

.... continued



STACK AND BLACK BOX MODULES





COMPOSITION CALCULATION MODULE

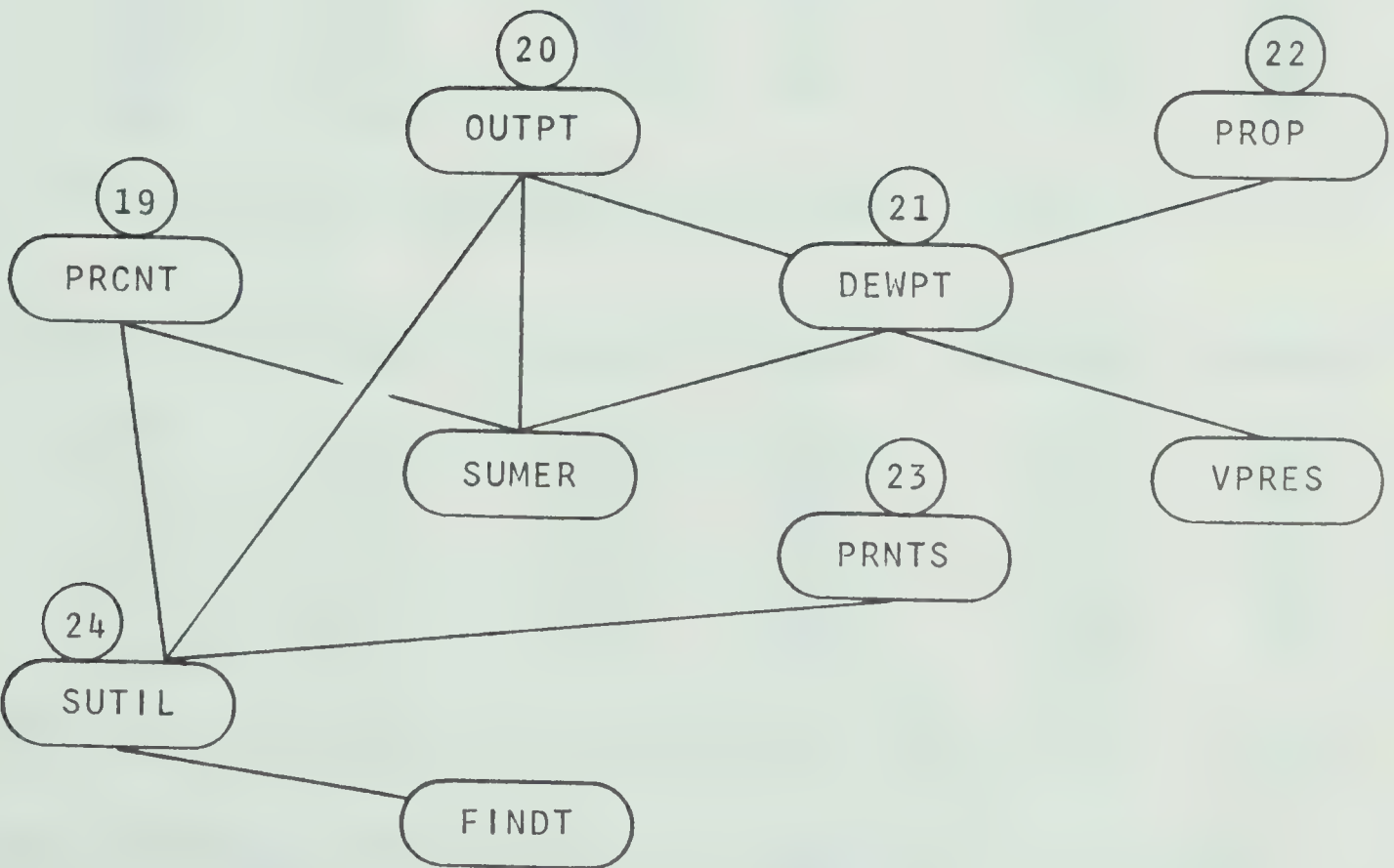


FIG. C-2 SUBROUTINE LINKAGES

PROG.NAME	STORAGE	PROG.NAME	STORAGE	PROG.NAME	STORAGE
MAIN	1032	SHIFT	1328	FLAGI	944
RCYCL	2712	MINFE	3520	FLAGJ	1792
TIMER	680	INIT	2104	NCALC	2760
PRINT	888	YMODY	1648	HLOSS	2256
FDSTM	944	GAUSS	1544	PDROP	1440
DSECT	1120	INPUT	2424	INLNB	704
OUTPT	4992	INPT0	2216	BRXNC	2528
SUTIL	1552	INPT1	2992	CNVTR	1024
PRNTS	1536	INPT2	3088	CRBED	1864
COMPR	776	INPT3	3384	DEWCK	1384
SETVU	336	INPT4	3120	CONDR	1888
HFCAL	1392	INPT5	2048	CINIT	2616
VPRES	1024	FFINP	4144	CINTG	2136
DEWPT	1552	SPECL	1856	CSECT	2144
FINDT	720	OPTIM	1272	CHBAL	1728
TCALC	2280	REDUC	4544	AQFND	1264
GUESR	672	DELTA	864	FOGST	2144
PROP	1464	EXCHN	1752	COMBN	1368
SUMER	928	DCHCK	1464	FINDE	1792
PRCNT	2552	FINSH	1280	CMBDV	1632
STEAM	1456	SEQNC	2000	AIRAD	2056
AIRFD	1680	RXWHB	2088	INCIN	3216
BKBOX	1120	BINIT	1896	STACK	3552
COMP	1944	DOPAS	1528	STAKU	2216
FAKER	576				

SUBROUTINE CORE REQUIREMENTS IN BYTES (TOTAL IS 135 K)

COMM.NAME	STORAGE	COMM.NAME	STORAGE	COMM.NAME	STORAGE
GEN1	80	EXEC1	408	HTLS1	32
GEN2	176	STOR1	5648	BURN1	32
DATA1	424	FLOW1	1508	BURN2	24
DATA2	320	INPUT1	416	COND1	108
DATA3	1120	INPUT2	220	STAK1	24
DATA4	240	OPT1	2816	STAK2	40
DATA5	184	OPT2	312	EXTRA	8

LABELLED COMMON CORE REQUIREMENTS IN BYTES (TOTAL IS 14 K)

TOTAL PROGRAM CORE REQUIREMENTS (INCLUDING I.B.M. 360/67 SYSTEM ROUTINES) ARE ABOUT 175 K BYTES.

TABLE C-1 PROGRAM CORE REQUIREMENTS

APPENDIX D

PROGRAM LISTING

ROUTINE	PAGE
-----	----

EXECUTIVE AND UTILITY ROUTINES

MAIN	D-3
RCYCL	D-5
TIMER	D-9
PRINT	D-10
FDSTM	D-11
DSECT	D-12
OUTPT	D-13
SUTIL	D-17
PRNTS	D-19
COMPR	D-21
SFTVU	D-22

AUXILIARY ROUTINES

HFCAL	D-23
VPRES	D-25
DEWPT	D-26
FINDT	D-29
TCALC	D-30
GUEFSR	D-33
PROP	D-35
SUMER	D-37
PRCNT	D-39
STEAM	D-42
AIRFD	D-44
BKBOX	D-46

COMPOSITION CALCULATION ROUTINES

COMP	D-48
SHIFT	D-51
MINFE	D-53
INIT	D-56
YMODY	D-59
GAUSS	D-62
FAKER	D-64

DATA INPUT ROUTINES

[illegible]

CALCULATION SEQUENCE OPTIMIZATION ROUTINES

[illegible]

EQUIPMENT MODULES ROUTINES

[illegible]


```

C *****
C *
C *          MAINLINE PROGRAM
C *
C * FUNCTIONS -
C *
C * - MAINLINE EXECUTIVE ROUTINE
C * - TRANSFERS CONTROL TO INPUT EXECUTIVE AND
C *   CALCULATION OPTIMIZATION EXECUTIVE
C * - INITIALIZES EQUIPMENT MODULE CALCULATIONS AND
C *   CALLS APPROPRIATE EQUIPMENT MODULE FOR THE
C *   CALCULATIONS FOR EACH EQUIPMENT UNIT IN
C *   THE FLOWSHEET
C * - CALLS CALCULATION SUMMARY ROUTINE WHEN
C *   PROCESS CALCULATIONS COMPLETED
C *
C *****

```

```

COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /EXEC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
$,ISUPR,IOPT
COMMON /STOR1/EQUIP(300),ILOCC,NMREQ,STREM(50,22)
$,NSIN(5),NSOUT(5)
COMMON /EXTRA/NDUMY,TDUMY
CALL TIMER
CALL INPUT
CALL TIMER
IF(IOPT) 29,29,30
29 CALL SEQNC
GO TO 31
30 CALL OPTIM
31 CALL TIMER
NDUMY=0
DO 150 I=1,25
IF(JTYPE(I)-1) 150,151,150
150 CONTINUE
GO TO 300
151 ILOCC=INDEX(I)+25
TDUM1=ABS(EQUIP(ILOCC))
WRITE(6,1000)
1000 FORMAT('0 NDUMY,TDUMY (I2,1X,F5.0)')
READ(5,1001,END=200) NDUMY,TDUMY
1001 FORMAT(I2,1X,F5.0)
200 TDUMY=SETVU(TDUMY,TDUM1)
WRITE(IWRIT,1002) TDUM1
1002 FORMAT(/T26,'PRIMARY REACTION CUT-OFF TEMPERATURE
$ (BOILER) ='F6.0
1,' DEG.F')
IF(NDUMY) 205,205,203
203 IDUMY=NGMS-NDUMY
WRITE(IWRIT,1003) TDUMY,IDUMY
1003 FORMAT(/T29,'SECONDARY REACTION CUT-OFF TEMPERATURE

```


MAINLINE PROGRAM ... (CONT'D)

```

$ = 'F6.0,
1' DFG.F'//T33'(BELOW THIS TEMPERATURE, THE LAST 'I2'
$ GASEOUS'/
2T34'MOLECULAR SPECIES ARE MASKED FOR THE BOILER'/T34
3'AND THE CONVERTER COMPOSITION CALCULATIONS.))'
205 WRITE(IWRIT,9000)
9000 FORMAT('0',T25,'*****')
$*****
1*****'/)
300 CONTINUE
    ISTAT=0
    NMBEQ=ISEQ(1)
21 ILOC=INDEX(NMBEQ)
    IEQIP=JTYPE(NMBEQ)
    CALL PRINT(IEQIP,NMBEQ)
    CALL FDSTM
    CALL DSECT (IEQIP)
    GO TO (1,2,3,4,5,6,7,8,9,10),IEQIP
1 CALL RXWHB
    GO TO 100
2 CALL INLNB
    GO TO 100
3 CALL CNVTR
    GO TO 100
4 CALL CONDR
    GO TO 100
5 CALL COMBN
    GO TO 100
6 CALL CMBOV
    GO TO 100
7 CALL AIRAD
    GO TO 100
8 CALL INCIN
    GO TO 100
9 CALL STACK
    GO TO 100
10 CALL BKBOX
100 CALL DSECT(IEQIP)
    CALL RCYCL(ISTAT)
    CALL TIMER
    IF(NMBEQ) 20,20,21
20 ITFST=IDBUG(15)
    CALL PRCNT(3)
    CALL OUTPT
    CALL TIMER
    WRITE(IWRIT,3000)
3000 FORMAT('1')
    CALL EXIT
    END

```



```

C *****
C *
C *          SUBROUTINE RCYCL
C *
C *  FUNCTIONS -
C *
C *  -  CALCULATION RECYCLE CONTROL ROUTINE
C *  -  DETECTS IF AND WHEN PROCESS CALCULATION
C *      RECYCLE IS REQUIRED
C *  -  RECYCLES CALCULATIONS WHEN ALL PREVIOUSLY
C *      ASSUMED STREAMS HAVE BEEN CALCULATED
C *  -  CHECKS FOR RECYCLE CALCULATION CONVERGENCE
C *      WHEN RECYCLE LOOP COMPLETED
C *  -  CONTROLS THE ACTIVE POSITION IN THE CALCULATION
C *      SEQUENCE VECTOR
C *
C *****

```

```

      SUBROUTINE RCYCL(ISTAT)
      DIMENSION ICALC(25),SSTOR(25,3)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /EXEC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
      $,ISUPR,IOPT
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STRFM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM

```

```

C*****      INITIALIZE IF AT BEGINNING OF CALCULATIONS

```

```

      IF(ISTAT) 400,400,402
400 DO 401 I=1,25
401 ICALC(I)=0
      IPNT0=1
      IPNT1=0
      IPLAC=1
      ISTAT=1
402 CONTINUE

```

```

C*****      IF NO STREAMS NEED BE ASSUMED, OMIT CHECKS.

```

```

      IF(IASUM(1)) 200,200,999

```

```

C*****      CHECK IF ANY INPUT STREAMS WERE ASSUMED.

```

```

      999 NSTRM=IASUM(IPNT1+1)
      IF(NSTRM) 2,2,101
101 NEQIP=INFO(NSTRM,3)
      IF(NMBEQ-NEQIP) 2,1,2
      1 IPNT1=IPNT1+1
      IF(IDBUG(15)-3) 999,810,810
      810 WRITE(IWRIT,2222) NSTRM
2222 FORMAT(T25' ASSUMED STREAM 'I3)

```


SUBROUTINE RCYCL ... (CONT'D)

GO TO 999

C***** CHECK IF ANY PREVIOUSLY ASSUMED STREAMS WERE
C***** CALCULATED.

```

2  IFLAG=0
   DO 3  IJ=IPNT0,IPNT1
     NSTRM=IASUM(IJ)
     IF(NSTRM) 200,200,102
102 NEQIP=INFO(NSTRM,2)
     IF(NEQIP-NMBEQ) 3,4,3
4   IFLAG=1
     ICALC(IJ)=1
     IF(IDBUG(15)-3) 3,311,811
811 WRITE(IWRIT,2223) NSTRM
2223 FORMAT(T25' CALCULATED STREAM 'I3)
3   CONTINUE
     IF(IFLAG) 200,200,100

```

C***** CHECK IF RECYCLE LOOP COMPLETED.

```

100 CONTINUE
    DO 10 IJ=IPNT0,IPNT1
      IF(ICALC(IJ)) 200,200,10
10  CONTINUE

```

C***** RECYCLE LOOP COMPLETE, CHECK CONVERGENCE.

```

    ICONV=1
    CRIT1=CRIT**0.5
    DO 50 IJ=IPNT0,IPNT1
      NSTRM=IASUM(IJ)
      IF(INFO(NSTRM,5)) 20,30,30
20  NEQIP=INFO(NSTRM,3)
      DO 25 I=2,6,2
        NUMBR=ABS(STREM(NSTRM,I-1))+0.5
        IF(NUMBR) 25,25,21
21  DVALU=ABS(STREM(NSTRM,I))+1.E-10
        IF(ABS(DVALU-SSTOR(IJ,I/2))/DVALU-CRIT1) 24,24,22
22  ICONV=0
24  SSTOR(IJ,I/2)=DVALU
        ILOC=INDEX(NEQIP)+NUMBR
        EQUIP(ILOC)=DVALU
25  CONTINUE
        GO TO 50
30  YTOT=0.0
        DO 31 I=1,NTOT
31  YTOT=YTOT+ABS(STREM(NSTRM,I))+1.E-10
        IF(ABS(YTOT-SSTOR(IJ,1))/YTOT-CRIT1) 33,33,32
32  ICONV=0

```


SUBROUTINE RCYCL ... (CONT'D)

```

33 SSTOR(IJ,1)=YTOT
   TEMP=ABS(STREM(NSTRM,21))+1.E-10
   IF(ABS(TEMP-SSTOR(IJ,2))/TEMP-CRIT1) 35,35,34
34 ICONV=0
35 SSTOR(IJ,2)=TEMP
   PRESS=ABS(STREM(NSTRM,22))+1.E-10
   IF(ABS(PRESS-SSTOR(IJ,3))/PRESS-CRIT1) 37,37,36
36 ICONV=0
37 SSTOR(IJ,3)=PRESS
50 CONTINUE
   IF(ICONV) 60,60,59

```

C***** RECYCLE LOOP CONVERGED, PROCEED PAST LOOP.

```

59 IPNT0=IPNT1+1
   GO TO 200

```

C***** RECYCLE LOOP NOT CONVERGED. PROCEED TO BEGINNING
C***** OF THE RECYLCE LOOP. (IE. LOOP)

```

60 NSTRM=IASUM(IPNT0)
   NMBEQ=INFO(NSTRM,3)
   ISTR=IPLAC
   DO 61 I=1,NNEQP
   IPLAC=I
   IF(ISEQ(I)-NMBEQ) 61,62,61
61 CONTINUE
   WRITE(IWRIT,5000)
62 CONTINUE
   DO 65 IJ=IPNT0,IPNT1
65 ICALC(IJ)=0
   IPNT1=IPNT0-1
   WRITE(IWRIT,1000) (ISEQ(I),I=IPLAC,ISTR)
   GO TO 900

```

C***** INCREMENT TO NEXT EQUIPMENT IN SEQUENCE VECTOR.

```

200 IPLAC=IPLAC+1

```

C***** CHECK FOR CALCULATIONS COMPLETE.

```

   IF(IPLAC-NNEQP) 201,201,202

```

C***** SET NEXT EQUIPMENT NUMBER TO BE DONE.

```

201 NMBEQ=ISEQ(IPLAC)
   GO TO 900

```

C***** FLAG CALCULATIONS COMPLETE.

SUBROUTINE RCYCL ... (CONT'D)

```
202 NMREQ=-1
900 CONTINUE
    RETURN
1000 FORMAT('0'T36'CALCULATIONS LOOPED ON RECYCLE LOOP -'/{
$ /T40,10I3))
5000 FORMAT('0 ERROR IN RECYCLE CONTROL')
    END
```



```

C  ****
C  *
C  *          SUBROUTINE TIMER
C  *
C  *  FUNCTIONS -
C  *
C  *  -  COMPUTING TIME MONITOR ROUTINE
C  *  -  OPTIONALLY ACTIVATED BY COMPILE TIME DATA FLAG
C  *  -  USES 360/67 OS SYSTEM TIMER ROUTINES
C  *      (CS019A AND CS019B)
C  *  -  OUTPUTS TIME INTERVAL SINCE LAST CALL AND
C  *      TOTAL COMPUTING TIME TO CALL
C  *
C  ****

```

```

      SUBROUTINE TIMER
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      DATA IFIRST, TOTIME / -2, 0.0 /
      IF(IFIRST) 3, 1, 2
1     CALL CS019A(IFIX(100.*1.E-6/26.))
      IFIRST=1
      RETURN
2     CALL CS019B(K)
      SEC=100.-FLOAT(K)/1.E-6*26.
      TOTIME=TOTIME+SEC
      WRITE(IWRIT,1000) SEC, TOTIME
      RETURN
3     IF(IFIRST+2) 5, 5, 4
4     WRITE(IWRIT,1234)
5     IFIRST=-1
      RETURN
1000 FORMAT('  T25' TIMER INTERVAL = 'F6.2' SEC., '
1     T62' TOTAL TIME = 'F6.2' SEC.' /)
1234 FORMAT('0')
      END

```



```

C  ****
C  *
C  *          SUBROUTINE PRINT
C  *
C  *  FUNCTIONS -
C  *
C  *  -  OUTPUT CONTROL ROUTINE
C  *  -  SETS OUTPUT PRIORITY FLAG FOR MODULE
C  *      CALCULATIONS BEFORE CONTROL IS TRANSFERRED BY
C  *      EXECUTIVE TO EQUIPMENT MODULE
C  *  -  IF 'PRINT SUPPRESS' OPTION IS USED,
C  *      CALCULATION OUTPUT IS SUPPRESSED FOR THE
C  *      FIRST PASS THROUGH RECYCLE LOOPS
C  *  -  CONTROLS INITIALIZATION OF PAGING FOR EACH
C  *      MODULE'S OUTPUT
C  *
C  ****

```

```

      SUBROUTINE PRINT(IEQIP,NMBEQ)
      DIMENSION IVEC(25)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /EXEC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
      $,ISUPR,IOPR
      COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
      DATA IVEC,ILINE/25*0,50/
      IF(ISUPR) 200,200,100
100  IF(IVEC(NMBEQ)) 104,104,101
101  ISUPR=1
      GO TO 200
104  IF(ISUPR-2) 105,900,900
105  DO 110 I=1,25
      IF(IASUM(I)) 110,110,106
106  NSTRM=IASUM(I)
      IF(INFO(NSTRM,3)-NMBEQ) 110,107,110
107  ISUPR=2
109  WRITE(IWRIT,1010)
      ILINE=0
      GO TO 900
110  CONTINUE
200  ITEST=IDBUG(IEQIP)*2
      IF(ITEST) 202,202,201
201  WRITE(IWRIT,1010)
      ILINE=50
      GO TO 203
202  ILINE=ILINE+4
      IF(ILINE-50) 203,203,109
203  RETURN
900  IVEC(NMBEQ)=1
      ITEST=0
      GO TO 202
1010 FORMAT('1'////)
      END

```



```

C *****
C *
C *          SUBROUTINE FDSTM
C *
C *  FUNCTIONS -
C *
C *  - EXECUTIVE UTILITY ROUTINE
C *  - FINDS STREAM INPUTS TO ACTIVE EQUIPMENT NUMBER
C *    AND STORES IN A VECTOR (NSIN) IN THE ORDER
C *    PROCESS, SERVICE, INFORMATION -- LATTER TWO
C *    FLAGGED NEGATIVE
C *  - FINDS STREAM OUTPUTS FROM ACTIVE EQUIPMENT
C *    NUMBER AND STORES IN A VECTOR (NSOUT) AS ABOVE
C *
C *****

```

```

      SUBROUTINE FDSTM
      DIMENSION I11111(3)
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      COMMON /STOR1/EQUIP(300), ILOC, NMBEQ, STREM(50,22)
      $, NSIN(5), NSOUT(5)
      COMMON /FLOW1/INFO(75,5), NNEQP, NOSTM
      DATA I11111/0,1,-1/
      NMAX=50
      ICNTI=0
      ICNTO=0
      DO 50 I=1,5
      NSIN(I)=0
50  NSOUT(I)=0
      ISIGN=+1
      DO 20 K=1,3
      ITST=I11111(K)
      DO 1 I=1,NMAX
      IF(INFO(I,5)-ITST) 1,2,1
      2 IF(INFO(I,3)-NMBEQ) 4,3,4
      3 ICNTI=ICNTI+1
      NSIN(ICNTI)=I*ISIGN
      GO TO 1
      4 IF(INFO(I,2)-NMBEQ) 1,5,1
      5 ICNTO=ICNTO+1
      NSOUT(ICNTO)=I*ISIGN
      1 CONTINUE
      ISIGN=-1
      20 CONTINUE
      IF(IDBUG(15)-5) 801,800,800
      800 WRITE(IWRIT,5000) (NSIN(I),I=1,ICNTI)
      WRITE(IWRIT,5001) (NSOUT(I),I=1,ICNTO)
      801 CONTINUE
      RETURN
5000 FORMAT('0 INPUT STREAMS ARE - ',5I3)
5001 FORMAT(' OUTPUT STREAMS ARE - ',5I3)
      END

```



```

C  ****
C  *
C  *          SUBROUTINE DSECT
C  *
C  *  FUNCTIONS -
C  *
C  *  - EXECUTIVE DEBUG OUTPUT ROUTINE
C  *  - OPTIONALLY DUMPS INPUT AND OUTPUT STREAMS AND
C  *    RELEVANT SECTION OF EQUIPMENT PARAMETER
C  *    VECTOR FOR ACTIVE EQUIPMENT NUMBER
C  *  - CALLED BEFORE AND AFTER EACH EQUIPMENT MODULE
C  *    CALCULATION
C  *  - OUTPUT RESULTS ONLY IF EXECUTIVE DEBUG FLAG
C  *    (IDBUG(15)) IS 4 OR GREATER
C  *
C  ****

```

```

      SUBROUTINE DSECT(IEQIP)
      DIMENSION ITYPE(10)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      DATA ITYPE/28,5,8,12,3,2,6,7,8,1/
      IF(IDBUG(15)-4) 801,800,800
800  CONTINUE
      ILOC1=ILOC+1
      ILOC2=ITYPE(IEQIP)+ILOC
      WRITE(IWRIT,9999) (EQUIP(J),J=ILOC1,ILOC2)
      IF(IDBUG(15)-5) 801,802,802
802  WRITE(IWRIT,9998)
      DO 1 I=1,5
        IF(NSIN(I)) 2,3,2
      2  J=IABS(NSIN(I))
        WRITE(IWRIT,9997) J,(STREM(J,K),K=1,NTOT),STREM(J,21)
        $,STREM(J,22)
      1  CONTINUE
      3  WRITE(IWRIT,9996)
      DO 10 I=1,5
        IF(NSOUT(I)) 12,801,12
      12 J=IABS(NSOUT(I))
        WRITE(IWRIT,9997) J,(STREM(J,K),K=1,NTOT),STREM(J,21)
        $,STREM(J,22)
      10 CONTINUE
801  CONTINUE
      RETURN
9999 FORMAT('0 EQUIP VECTOR SEGMENT -'/((' ',10E11.4))
9998 FORMAT('0 INPUT STREAMS ARE -' )
9997 FORMAT(' ',I3/(((' ',10E11.4))
9996 FORMAT('0 OUTPUT STREAMS ARE -' )
      END

```



```

C *****
C *
C *          SUBROUTINE OUTPT
C *
C *  FUNCTIONS -
C *
C *  -  PROCESS CALCULATION SUMMARY OUTPUT ROUTINE
C *  -  OUTPUTS SUMMARY RESULTS IF EXECUTIVE OUTPUT
C *      FLAG (IDBUG(15)) IS 1 OR GREATER
C *  -  OUTPUTS 'OVER ALL PLANT MASS AND ENERGY
C *      BALANCES', 'EQUIPMENT PARAMETER SUMMARY' AND
C *      'STREAM COMPOSITION AND PROPERTY SUMMARY'
C *      WHEN ALL PROCESS CALCULATIONS ARE COMPLETE
C *
C *****

```

```

      SUBROUTINE OUTPT
      DIMENSION CMTRX(20,5),TOT1(5),TOT2(5),TOT3(5),TOT4(5)
      $,ENTH(5),
      IVOL(5),TDEGF(5),TDEW(5),PSIA(5),NSTRM(5),YCOMP(20)
      DIMENSION ISPEC(30),PVEC(30),ITYPE(10)
      DIMENSION R1(5),R2(5),R3(5),R4(5),R5(5),R6(5),R7(5),
      1R8(5),R9(5),R10(5),RN(5,10)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /DATA2/NAME(20,4)
      COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(5),VMOLE(20)
      COMMON /EXEC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
      $,ISUPR,IOPT
      COMMON /STOR1/EQUIP(300),ILCC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
      EQUIVALENCE (R1(1),RN(1,1)),(R2(1),RN(1,2))
      1,(R3(1),RN(1,3)),(R4(1),RN(1,4)),(R5(1),RN(1,5))
      1,(R6(1),RN(1,6)),(R7(1),RN(1,7)),(R8(1),RN(1,8))
      1,(R9(1),RN(1,9)),(R10(1),RN(1,10))
      DATA R1/'      W','ASTE',' HFA','T BO','ILER'/
      DATA R2/'      ',' IN','-LIN','E BU','RNER'/
      DATA R3/'      ','      ','      C','ONVF','RTER'/
      DATA R4/'      ','      ','      C','ONDE','NSER'/
      DATA R5/'      AD','IABA','TIC ','COMB','INER'/
      DATA R6/'      ','COMB','INER','/DIV','IDER'/
      DATA R7/'COMB','USTI','ON A','IR A','DDER'/
      DATA R8/'      ','      ','      INC','INER','ATOR'/
      DATA R9/'      ','      ','      ','      S','TACK'/
      DATA R10/'      ','      ','      B','LACK',' BOX'/
      DATA ITYPE/28,5,8,12,3,2,6,7,8,1/
      DATA ISTAR,IBLNK,HUGE/'* ','      ','1.E30/
      IF(ITEST-1) 900,800,800
800 CONTINUE
      ITEST=0
      ILINE=11
      WRITE(IWRIT,1000)

```


SUBROUTINE OUTPT ... (CONT'D)

```

WRITE(IWRIT,9000)
WRITE(IWRIT,1010)
WRITE(IWRIT,9000)
DO 1 IJK=1,NNEQP
  NMBEQ=ISEQ(IJK)
  ILOC=INDEX(NMBEQ)
  IEQIP=JTYPE(NMBEQ)
  INUMB=ITYPE(IEQIP)
  DO 2 I=1,INUMB
    IPLAC=ILOC+I
    VALUE=EQUIP(IPLAC)
    ISPEC(I)=IBLNK
    IF(VALUE) 3,4,4
  3 ISPEC(I)=ISTAR
  4 PVEC(I)=ABS(VALUE)
  2 CONTINUE
  ICHEK=(INUMB+1)/2+4
  IF(ILINE+ICHEK-54) 6,6,5
  5 WRITE(IWRIT,1000)
  WRITE(IWRIT,9000)
  WRITE(IWRIT,1010)
  WRITE(IWRIT,9000)
  ILINE=11
  6 ILINE=ILINE+ICHEK
  WRITE(IWRIT,1001) NMBEQ,(RN(J,IEQIP),J=1,5),
  1 (J,PVEC(J),ISPEC(J),J=1,INUMB)
  1 CONTINUE
  WRITE(IWRIT,9000)
  IND=1
  DO 100 KK=1,50
    IF(INFO(KK,5)) 98,15,15
  15 NSTRM(IND)=INFO(KK,1)
    IF(NSTRM(IND)) 98,98,10
  10 IF(IND-5) 20,300,300
  20 IF(KK-50) 30,300,300
  30 IND=IND+1
  GO TO 100
  300 IF(NSTRM(1)) 100,100,303
  303 WRITE(IWRIT,2000)
  WRITE(IWRIT,9000)
  WRITE(IWRIT,2020)
  WRITE(IWRIT,9000)
  WRITE(IWRIT,2001) (NSTRM(I),I=1,IND)
  DO 301 J=1,IND
    CALL SUTIL(NSTRM(J),1,YCOMP,TEMP,PRESS)
  DO 302 I=1,NTOT
  302 CMTRX(I,J)=YCOMP(I)
  CALL SUMER(YCOMP,NTOT,0,TOT1(J),TOT2(J))
  CALL SUMER(YCOMP,NGMS,0,TOTAL,TMASS)
  CALL SUMER(YCOMP,NTOT,1,DUMY,TOT3(J))

```


SUBROUTINE OUTPT ...(CONT'D)

```

      CALL SUMER(YCOMP,NTOT,2,DUMY,TOT4(J))
      ENTH(J)=HUGE
      VOL(J)=HUGE
      IF(TOT1(J)-1.0E-6) 310,310,304
304  IF(YCCMP(IDH2O)-0.1) 309,309,305
305  IF(ABS(YCOMP(IDH2O)-TOT1(J))/YCOMP(IDH2O)-0.01) 310
      $,309,309
309  ENTH(J)=HFCAL(TEMP,YCOMP,0)*1.0E-6
      IF(TOTAL-1.E-6) 310,310,306
306  VOL(J)=TOTAL/60.*10.73*(TEMP+459.69)/PRESS
310  TDEGF(J)=TEMP
      TDEW(J)=0.0
      IF(TOTAL-1.0E-4) 312,311,311
311  TDEW(J)=500.
      CALL DEWPT(TDEW(J),YCOMP,PRESS,1)
312  PSIA(J)=PRESS
301  CONTINUE
      DO 400 I=1,NTOT
400  WRITE(IWRIT,2002) (NAME(I,J),J=1,4),(CMTRX(I,J),J=1
      $,IND)
      WRITE(IWRIT,2003) (TOT1(I),I=1,IND)
      WRITE(IWRIT,2004) (TOT2(I),I=1,IND)
      WRITE(IWRIT,2005) (TOT3(I),I=1,IND)
      WRITE(IWRIT,2015) (TOT4(I),I=1,IND)
      WRITE(IWRIT,2006) (ENTH(I),I=1,IND)
      WRITE(IWRIT,2007) ( VOL(I),I=1,IND)
      WRITE(IWRIT,2008) (TDEGF(I),I=1,IND)
      WRITE(IWRIT,2009) ( TDEW(I),I=1,IND)
      WRITE(IWRIT,2010) ( PSIA(I),I=1,IND)
      WRITE(IWRIT,9000)
      IND=1
      NSTRM(1)=0.0
      GO TO 100
98  IF(KK-50) 100,99,99
99  IND=IND-1
      GO TO 300
100  CONTINUE
900  CONTINUE
      RETURN
1000  FORMAT('1'////T41'EQUIPMENT PARAMETER SUMMARY')
1010  FORMAT(T36'PARAMETER NUMBERS AND PARAMETER VALUES'
      1/T33, '( '*' DENOTES PARAMETER VALUE SPECIFICATION)')
1001  FORMAT(//T25'EQUIPMENT NUMBER'I3,T65,5A4,/(T30,I3,
      1' = ',F13.6,1X,A1,8X,I3,' = 'F13.6,1X,A1))
2000  FORMAT('1'////T35'STREAM COMPOSITION AND PROPERTY
      $ SUMMARY.')
2020  FORMAT(T25
      1'UNITS ARE -'T62'COMPOSITION - MOLES/HR.'/T25'ENTHALPY
      $ - MMBTU./HR
      1.'T54'VOLUME - CU.FT./MIN. (GAS ONLY)'/T25'TEMPERATURE

```


SUBROUTINE OUTPT ...{CONT'D}

```

$ - DEG.F.'
1T69'PRESSURE - PSIA.')
```

2001	FORMAT (T25'STREAM NO.'
2002	FORMAT(T25,4A1,6X,5F10.4)
2003	FORMAT('0'T25'TOT. MOLES',5F10.3)
2004	FORMAT('0'T25'TOT. LBS. '5F10.1)
2005	FORMAT(T25'TOT.LB.S(M)'F9.1,4F10.1)
2015	FORMAT(T25'TOT.LB.S(E)'F9.1,4F10.1)
2006	FORMAT('0'T25'ENTHALPY '5(2X,F3.3))
2007	FORMAT(T25'VOLUME '5(2X,F8.1))
2008	FORMAT('0'T25'TEMPERATURE'F9.2,4F10.2)
2009	FORMAT(T25'S. DEW PT.'5F10.2)
2010	FORMAT(T25'PRESSURE '5F10.2)
9000	FORMAT('0',T25,'*****')

```

$*****
1*****')/)
```

END


```

C  ****
C  *
C  *          SUBROUTINE SUTIL
C  *
C  *  FUNCTIONS -
C  *
C  *  -  STREAM STORAGE UTILITY ROUTINE
C  *  -  DEPENDING UPON A FLAG, STORES A STREAM IN
C  *      STREAM MATRIX (STREM), RETRIEVES A STREAM
C  *      FROM STREAM MATRIX, OR COMBINES ALL INPUT
C  *      STREAMS (WITH OPTIONAL EXCLUSION OF ONE
C  *      INPUT STREAM) TO ACTIVE EQUIPMENT NUMBER.  IN
C  *      LAST CASE, RESULTING TEMPERATURE AND
C  *      PRESSURE ARE FOUND
C  *
C  ****

```

```

      SUBROUTINE SUTIL(NSTRM,IDO,YDUMY,TDUMY,PDUMY)
      DIMENSION YDUMY(20),YEXTR(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      IF(IDO-1) 100,101,102
100  DO 12 I=1,NTOT
      12 YDUMY(I)=0.0
      ENTH=0.0
      PDUMY=100.
      NOTSN=NSTRM
      DO 1 I=1,5
      NSTRM=IABS(NSIN(I))
      IF(NSIN(I)) 6,6,2
      2 IF(NSIN(I)-NOTSN) 3,1,3
      3 DO 4 J=1,NTOT
      YEXTR(J)=ABS(STREM(NSTRM,J))
      YDUMY(J)=YDUMY(J)+YEXTR(J)
      4 CONTINUE
      TDUMY=ABS(STREM(NSTRM,21))
      ENTH=ENTH+HFCAL(TDUMY,YEXTR,0)
      PTEST=ABS(STREM(NSTRM,22))
      IF(PTEST) 1,1,5
      5 PDUMY=AMIN1(PDUMY,PTEST)
      1 CONTINUE
      6 CALL FINDT(YDUMY,TDUMY,ENTH)
      RETURN
101  IF(NSTRM) 105,105,104
105  DO 60 I=1,NTOT
      60 YDUMY(I)=0.0
      PDUMY=0.0
      TDUMY=0.0
      RETURN
104  DO 40 I=1,NTOT

```


SUBROUTINE SUTIL ... (CONT'D)

```
40 YDUMY(I)=ABS(STREM(NSTRM,I))
   TDUMY=ABS(STREM(NSTRM,21))
   PDUMY=ABS(STREM(NSTRM,22))
   RETURN
102 IF(NSTRM) 107,107,106
106 DO 50 I=1,NTOT
   50 STREM(NSTRM,I)=SIGN(YDUMY(I),STREM(NSTRM,I))
      STREM(NSTRM,21)=SIGN(TDUMY,STREM(NSTRM,21))
      STREM(NSTRM,22)=SIGN(PDUMY,STREM(NSTRM,22))
107 RETURN
   END
```



```

C *****
C *
C *          SUBROUTINE PRNTS
C *
C * FUNCTIONS -
C *
C * - STREAM OUTPUT UTILITY ROUTINE
C * - OUTPUT RESULTS ONLY IF PRESENT OUTPUT
C *   PRIORITY FLAG IS 1 OR GREATER
C * - OUTPUTS EQUIPMENT PROCESS FEED (COMBINED),
C *   PRESENT ACTIVE STREAM (YCOMP), OR STREAM FROM
C *   STREAM MATRIX, DEPENDING UPON A FLAG
C * - TEMPERATURE, PRESSURE, ENTHALPY AND MOLE
C *   NUMBERS OF STREAM CONSTITUTE OUTPUT
C *
C *****

```

```

      SUBROUTINE PRNTS(INDIC)
      DIMENSION YDUMY(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /DATA2/NAME(20,4)
      IF(ITEST-1) 20,10,10
20  RETURN
10  CONTINUE
      IF(INDIC) 1,2,3
      1  WRITE(IWRIT,9000)
         WRITE(IWRIT,1000)
         WRITE(IWRIT,1001) TFEED,PRESS
         WRITE(IWRIT,8013) ENTH,((NAME(I,J),J=1,4),YFEED(I),I=1
         $,NTOT)
         GO TO 900
      2  IF(ITEST-1) 900,21,21
21  WRITE(IWRIT,8000)
         WRITE(IWRIT,8013) ENTH,((NAME(I,J),J=1,4),YCOMP(I),I=1
         $,NTOT)
         GO TO 900
      3  NSTRM=INDIC
         CALL SUTIL(NSTRM,1,YDUMY,TDUMY,PDUMY)
         DENTH=HFCAL(TDUMY,YDUMY,0)
         WRITE(IWRIT,2000) NSTRM
         WRITE(IWRIT,1001) TDUMY,PDUMY
         WRITE(IWRIT,8013) DENTH,((NAME(I,J),J=1,4),YDUMY(I)
         $,I=1,NTOT)
      900 WRITE(IWRIT,9000)
         RETURN
1000 FORMAT(T44,'EQUIPMENT PROCESS FEED'/)
1001 FORMAT(T25,'TEMPERATURE (DEG. F) = ',F7.1,T61
         $,'PRESSURE (PSIA) = '
         1,F6.2)
2000 FORMAT(T47,'STREAM NUMBER',I3/)
8000 FORMAT(' ')

```


SUBROUTINE PRNTS ... (CONT'D)

```
8013 FORMAT( T35, 'STREAM ENTHALPY (BTU.) = ', E15.7// T46  
$, 'MOLE NUMBERS  
1ARE -'// (T29, 4A1, ' - ', F15.5, 10X, 4A1, ' - ', F15.5))  
9000 FORMAT('O', T25, '*****  
$*****  
1*****' / )  
END
```



```

C *****
C *
C *          SUBROUTINE COMPR
C *
C *  FUNCTIONS -
C *
C *  - DATA COMPATIBILITY CHECK UTILITY ROUTINE
C *  - COMPARES A STREAM PARAMETER (PARAMETER NSPAR
C *    OF STREAM NSTRM) WITH AN EQUIPMENT PARAMETER
C *    (PARAMETER NEPAR OF ACTIVE EQUIPMENT NUMBER)
C *  - IF ONE IS ZERO, THE TWO VALUES ARE EQUATED TO
C *    THE NEGATIVE SPECIFICATION VALUE
C *  - IF TWO VALUES ARE DIFFERENT (AND NON-ZERO) AN
C *    ERROR MESSAGE RESULTS -- BOTH VALUES ARE
C *    EQUATED TO EQUIPMENT PARAMETER VALUE
C *
C *****

```

```

      SUBROUTINE COMPR (NSTRM,NSPAR,NEPAR)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      IF(NSTRM) 900,900,100
100  NLOC=NEPAR+ILOC
      SVALU=STREM(NSTRM,NSPAR)
      EVALU=EQUIP(NLOC)
      IF(SVALU*EVALU) 1,2,3
      1  WRITE(IWRIT,1000) NSTRM,NSPAR,NMBEQ,NEPAR
      2  IF(EVALU) 10,12,12
10   STREM(NSTRM,NSPAR)=EVALU
      GO TO 900
12  EQUIP(NLOC)=SVALU
      GO TO 900
      3  IF(ABS(SVALU-EVALU)-ABS(SVALU/1000.)) 900,900,1
900  RETURN
1000 FORMAT('O  CONFLICTING DATA GIVEN - '/'  NSTRM = ',I4
      $,'  NSPAR = '
      1,I4,'  NMBEQ = ',I4,'  NEPAR = ',I4)
      END

```



```

C *****
C *
C *          FUNCTION SETVU
C *
C * FUNCTIONS -
C *
C * - DEFAULT VALUE UTILITY FUNCTION
C * - CHECKS A TEST VALUE -- IF POSITIVE, FUNCTION
C *   IS SET TO TEST VALUE
C * - IF TEST VALUE IS ZERO OR NEGATIVE, FUNCTION
C *   IS SET TO DEFAULT VALUE
C *
C *****

```

```

      FUNCTION SETVU(TEST,VALUE)
      IF(TEST) 3,3,4
3     TEST=VALUE
4     SETVU=TEST
      RETURN
      END

```



```

C *****
C *
C *          FUNCTION HFCAL
C *
C * FUNCTIONS -
C *
C * - THERMODYNAMIC PROPERTY EVALUATION ROUTINE
C * - FOR GIVEN STREAM MOLE NUMBERS AND TEMPERATURE,
C *   EVALUATES (DEPENDING UPON A FLAG)--
C *   - TOTAL STREAM HEAT CAPACITY, OR
C *   - TOTAL STREAM ENTHALPY, OR
C *   - ONE MOLECULAR SPECIE'S FREE ENERGY FUNCTION
C *
C *****

```

```

FUNCTION HFCAL (TF,Y,J)
DIMENSION Y(20)
COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /DATA3/TDATA(20,14)

```

```

C*****      Y - STREAM MOLE NUMBERS
C*****      TF - TEMPERATURE, DEG. FAHRENHEIT
C*****      J - THERMODYNAMIC PROPERTY FLAG
C*****      = -VE - STREAM HEAT CAPACITY CALCULATED,
C*****              (BTU./LB.MOLE DEG. F)
C*****      = 0   - STREAM ENTHALPY CALCULATED (BTU.)
C*****              (RELATIVE NOT ABSOLUTE)
C*****      = +VE - DIMENSIONLESS FREE ENERGY FUNCTION,
C*****              (F/RT), FOR JTH MOLECULAR SPECIE
C*****              CALCULATED.
C*****
C*****      CONVERT TEMPERATURE FROM FAHRENHEIT TO KELVIN FOR
C*****      CALCULATIONS

```

```

TK=(TF+459.69)/1.8

```

```

C*****      DECIDE WHAT DATA TO USE
C*****      FOR (300. - 1000. DEG.K) , K=0
C*****      USE TDATA(-,1) TO TDATA(-,7)
C*****      FOR (1000. - 5000. DEG K) , K=7
C*****      USE TDATA(-,8) TO TDATA(-,14)

```

```

      K=0
      IF(TK-1000.) 1,1,2
2 K=7
1 CONTINUE
      IF(J) 100,200,300

```

```

C*****      CALCULATE HEAT CAPACITY (BTU/LB.MOLE.DEG.F)

```

```

100 YTOT=0.
      SUM=0.

```


FUNCTION HFCAL ... (CONT'D)

```

DO 10 I=1,NTOT
  SUM=SUM+(TDATA(I,K+1)+TDATA(I,K+2)*TK+TDATA(I,K+3)
1  *TK**2+TDATA(I,K+4)*TK**3+TDATA(I,K+5)*TK**4)*Y(I)
  YTOT=YTOT+Y(I)
10 CONTINUE

```

C***** EQUATE 'HFCAL' TO THE HEAT CAPACITY

```

HFCAL=SUM*1.98726/YTOT
GO TO 900

```

C***** CALCULATE RELATIVE STREAM ENTHALPY (BTU.)

```

200 SUM=0.
DO 20 I=1,NTOT
  SUM=SUM+(TDATA(I,K+1)+TDATA(I,K+2)/2.*TK+TDATA(I,K+3)
1  /3.*TK**2+TDATA(I,K+4)/4.*TK**3+TDATA(I,K+5)/5.*TK**4
1  +TDATA(I,K+6)/TK)*Y(I)
20 CONTINUE

```

C***** EQUATE 'HFCAL' TO THE STREAM ENTHALPY

```

HFCAL = SUM*1.98726*TK*1.8
GO TO 900

```

C***** CALC. FREE ENERGY FUNCTION (F/RT) FOR JTH SPECIE
 C***** EQUATE TO 'HFCAL'

```

300 HFCAL=TDATA(J,K+1)*(1.-ALOG(TK))-TDATA(J,K+2)/2.*TK
1  -TDATA(J,K+3)/6.*TK**2-TDATA(J,K+4)/12.*TK**3
1  -TDATA(J,K+5)/20.*TK**4+TDATA(J,K+6)/TK-TDATA(J,K+7)
900 RETURN
END

```



```

C *****
C *
C *          SUBROUTINE VPRES
C *
C *  FUNCTIONS -
C *
C *  -  VAPOR PRESSURE CALCULATION ROUTINE
C *  -  DEPENDING UPON A FLAG, CALCULATES WATER OR
C *      SULPHUR VAPOR PRESSURE AT A GIVEN TEMPERATURE
C *      (ALSO FIRST DERIVATIVE OF VAPOR PRESSURE
C *      W. R. T. TEMPERATURE)
C *
C *****

```

```

      SUBROUTINE VPRES(PCALC,DP,TF,IFLAG)

```

```

C*****      CONVERT FROM FAHRENHEIT TO KELVIN

```

```

      TK=(TF+459.69)/1.8

```

```

      IF(IFLAG) 10,10,20

```

```

C*****      CALCULATE WATER VAPOR PRESS. AND DERATIVE AT TK.

```

```

C*****      REF. KEENAN AND KEYS (50 - 374.11 DEG. C)

```

```

10 X=647.27-TK

```

```

      V=X/TK

```

```

      U=3.3463130+4.14113E-2*X+ 7.515484E-9*X**3+6.56444E-11

```

```

      $*X**4

```

```

      W=1+1.3794481E-2*X

```

```

      DV=-647.27/TK**2

```

```

      DW=-1.3794481E-2

```

```

      DU=-(4.14113E-2+3.* 7.515484E-9*X**2+4.*6.56444E-11*X*
      $*3)

```

```

      PCALC=218.167*EXP(-2.303*(V*U/W))

```

```

      DP=-PCALC*2.303*(V*(W*DU-U*DW)/W**2+U*DV/W)

```

```

      GO TO 30

```

```

C*****      CALCULATE SULPHUR VAPOR PRESS. AND DERIV. AT TK

```

```

C*****      REF. TEXAS GULPH SULPHUR DATA BOOK

```

```

20 IF(TK-700) 21,22,22

```

```

C*****      SHOULD BE 600. (CONVERGENCE PROBLEMS)

```

```

21 PCALC=EXP((14.7-.0062238*TK-5405.1/TK)*2.303)/760.0

```

```

      DP=PCALC*2.303*(-0.0062238+5405.1/TK**2)

```

```

      GO TO 30

```

```

22 PCALC=EXP((7.43287-3268.2/TK)*2.303)/760.0

```

```

      DP=PCALC*2.303*(3268.2/TK**2)

```

```

30 RETURN

```

```

      END

```



```

C  ****
C  *
C  *          SUBROUTINE DEWPT
C  *
C  *  FUNCTIONS -
C  *
C  *  -  DEW POINT CALCULATION ROUTINE
C  *  -  DEPENDING UPON A FLAG, CALCULATES WATER OR
C  *      SULPHUR DEW POINT (USING NEWTON'S METHOD) FOR
C  *      GIVEN PRESSURE AND STREAM MOLE NUMBERS
C  *  -  REQUIRES AN INITIAL ESTIMATE OF DEW PT. TEMP.
C  *
C  ****

```

```

      SUBROUTINE DEWPT (TF,Y,PSPEC,IFLAG)
      DIMENSION Y(20)
      COMMON /GFN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMDLE(20)
      IF(ITEST-9) 811,810,810
      810 WRITE(IWRIT,9999)
      9999 FORMAT(1H0,' DEW POINT CALCULATION  ''DEWPT''
      $          '/')
      811 CONTINUE

```

```

C*****      IFLAG = 0  - WATER DEW POINT CALCULATION
C*****      = 1  - SULPHUR DEW POINT CALCULATION
C*****
C*****      FIND TOTAL NUMBER OF MOLES IN STREAM FOR
C*****      SUBSEQUENT MOLE FRACTION DETERMINATION

```

```

      CALL SUMER(Y,NGMS,0,YTOT,DUMY)

```

```

C*****      FIND MOLE FRACTION (YFRAC) WATER OR SULPHUR, USING
C*****      COMPONENT IDENTIFICATIONS (IDH2O,IDSUL)

```

```

      IF(IFLAG) 2,2,3

```

```

C*****      WATER MOLE FRACTION

```

```

      2 YFRAC=Y(IDH2O)/YTOT
      GO TO 4

```

```

C*****      SULPHUR MOLE FRACTION (5 SULPHUR SPECIES MAXIMUM)
C*****      CHECK GIVEN TEMP TO SEE WHAT COMP. TO USE FOR MOLE
C*****      FRACTION DETERMINATION. (SULPHUR)

```

```

      3 IF(TF-700.0) 10,10,20

```

```

C*****      TEMP. IS BELOW 700.0 DEG. F. - USE GIVEN
C*****      COMPOSITION.

```

```

      10 CALL SUMER(Y,NGMS,1,STOT,DUMY)

```


SUBROUTINE DEWPT ...(CONT'D)

```
YFRAC=STOT/YTOT
GO TO 4
```

```
C***** TEMP. IS ABOVE 700. DEG.F.
C***** ASSUME ALL SULPHUR (GAS) IN S8 FORM AT DEW POINT
C***** - (IF. CONVERT ALL GASEOUS SULPHUR FORMS IN GIVEN
C***** STREAM TO S8 EQUIVALENT).
```

```
20 CALL SUMFR(Y,NGMS,1,DUMY,SMASS)
YFRAC=SMASS/(32.0*8.0*YTOT)
```

```
C***** USE GIVEN TEMPERATURE AS INITIAL GUESS IN
C***** ITERATIVE CALCULATION OF DEW POINT. NEWTON'S
C***** METHOD IS USED - (IF. AT EACH TEMP. GUESSED,
C***** CALCULATE VAPOR PRESSURE AND DERIVATIVE W.R.T.
C***** TEMP. CORRECT TEMPERATURE RESULTS IN VAPOR
C***** PRESSURE EQUALLING PARTIAL PRESSURE OF COMPONENT
C***** - IDEAL GAS BEHAVIOR ASSUMED - DALTON'S LAW
C***** USED.
C*****
C***** CALCULATE PARTIAL PRESSURE AND ERROR RESULTING FROM
C***** GUESSED TEMPERATURE.
C***** IF MOLE FRACTION IS ZERO, SET DEW PT. TO 0.0
```

```
4 IF(YFRAC-1.0E-6) 100,100,30
100 TF=0.0
GO TO 40
30 IF(TF-200.) 31,31,5
31 TF=500.
5 CALL VPRES(PCALC,DP,TF,IFLAG)
PARTP=PSPEC/14.696*YFRAC
ERROR=PARTP-PCALC
IF(ITEST-9) 801,800,800
800 WRITE(IWRIT,5001) TF,YFRAC,PCALC,PARTP,ERROR,DP
801 CONTINUE
TF=TF+ERROR/DP*1.8
```

```
C***** CHECK FOR CONVERGENCE - IF ERROR SUFFICIENTLY
C***** SMALL, TERMINATE - OTHERWISE ITERATE WITH NEW
C***** TEMP.
```

```
IF(ABS(ERROR/PSPEC*14.696)-CRIT)40,40,5
40 CONTINUE
IF(ITEST-5)803,802,802
802 IF(IFLAG) 804,804,805
804 WRITE(IWRIT,5000) PARTP,TF,CRIT
GO TO 803
805 WRITE(IWRIT,5002) PARTP,TF,CRIT
803 CONTINUE
RETURN
```


SUBROUTINE DEWPT ...(CONT'D)

```
5000 FORMAT(1H0,'WATER DEW POINT FOR PARTIAL PRESSURE OF '  
$,F10.4,' ATM.  
1      IS 'F10.4,' DEG. F'/'      ( CRIT = ',E9.2' )' )  
5001 FORMAT(1H0,      '      TF = ',F15.7,2X,'YFRAC = '  
$,E15.7,2X,  
1'PCALC = ',F15.7,/1X,'PARTP = ',F15.7,2X,'ERROR = '  
$,E15.7,2X,  
1'      DP = ',F15.7)  
5002 FORMAT(1H0,'SULPHUR DEW POINT FOR PARTIAL PRESSURE OF  
$ ',F10.4,' AT  
1M.      IS 'F10.4,' DEG. F'/'      ( CRIT = ',E9.2'  
$ )' )  
      END
```



```

C *****
C *
C *          SUBROUTINE FINDT
C *
C *  FUNCTIONS -
C *
C *  - TEMPERATURE CALCULATION ROUTINE
C *  - GIVEN STREAM MOLE NUMBERS AND A REFERENCE
C *    ENTHALPY, FINDS THE CORRESPONDING TEMPERATURE
C *    ASSUMING NO COMPOSITION CHANGES (NEWTON'S
C *    METHOD USED)
C *  - REQUIRES AN INITIAL ESTIMATE OF TEMPERATURE
C *
C *****

      SUBROUTINE FINDT(YCOMP,TEMP,ENTHR)
      DIMENSION YCOMP(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      YTOT=0.0
      DO 10 I=1,NTOT
10  YTOT=YTOT+YCOMP(I)
      1  ENTH=HFCAL(TEMP,YCOMP,0)
      DHDT=HFCAL(TEMP,YCOMP,-1)*YTOT
      ERROR=ENTH-ENTHR
      TEMP=TEMP-ERROR/DHDT
      IF( ITEST -9) 801,800,800
800  WRITE(IWRIT,1000) TEMP,ENTH,ERROR
801  CONTINUE
      IF(ABS(ERROR/ENTHR)-CRIT) 2,2,1
      2  RETURN
1000  FORMAT(' (FINDT) - TEMP = ',E11.4,' ENTH = ',E11.4,'
$  ERROR = ',
1E11.4)
      END

```



```

C *****
C *
C *          SUBROUTINE TCALC
C *
C *  FUNCTIONS -
C *
C *  -  ITERATIVE TEMPERATURE DETERMINATION ROUTINE
C *  -  FOR A GIVEN FEED STREAM, FINDS ADIABATIC OR
C *  -  NON-ADIABATIC TEMPERATURE, DEPENDING ON A FLAG
C *  -  TAKES INTO ACCOUNT COMPOSITION CHANGES WITH
C *  -  TEMPERATURE
C *  -  FOR NON-ADIABATIC CASE (BOILER), HEAT LOSS
C *  -  IS EVALUATED USING MEAN STREAM PROPERTIES
C *  -  (ALSO PRESSURE DROP IS CALCULATED AND REDUCED
C *  -  PRESSURE IS USED FOR OUTLET COMPOSITION
C *  -  CALCULATION)
C *  -  TCTOF (EQUIL. CUTOFF TEMP.) MUST BE PREVIOUSLY
C *  -  SET
C *  -  RIGOR OF CALCULATIONS INITIALLY IS LOW, BUT IS
C *  -  INCREASED AS CONVERGENCE (USING SECANT METHOD)
C *  -  IS ACHIEVED
C *  -  INITIAL POSITIVE SET IS GENERATED FOR FIRST
C *  -  TEMPERATURE ESTIMATES, BUT THIS GENERATION IS
C *  -  BYPASSED WHEN CONVERGENCE IS NEARLY ACHIEVED
C *  -  REQUIRES AN INITIAL ESTIMATE (TEMP)
C *
C *****

```

```

      SUBROUTINE TCALC(NOHLS)
      DIMENSION YAVG(20)
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      COMMON /GEN2/TEMP, TFEED, YCOMP(20), YFEED(20), PRESS, ENTH
      COMMON /HTLS1/TNUMB, TDIAM, TLONG, TSHL1, TSHL2, QLOSS
      $, DELPC, DELTP
      COMMON /BURN2/IFLAG, IPASS, MPASS, ESTMT(3)
      DATA TWALL/500./

```

```

C*****      CALCULATE REFERENCE ENTHALPY OF INLET STREAM AT
C*****      INLET TEMP.

```

```

      ENTHR=HFCAL(TFEED,YFEED,0)
      IF(ITEST-3) 811,810,810
810 WRITE(IWRIT,5010) TFEED,ENTHR
811 CONTINUE
      DELPC=0.0
      IFNSH=0
      ITERH=0
      KINIT=1
      LOOSE=0

```

```

C*****      GENERATE A TEMPERATURE GUESS.

```


SUBROUTINE TCALC ...(CONT'D)

```

1 CONTINUE
  FAC1=1.01+(1-LOOSE)*0.09
  FAC2=1.0
  CALL GUESR(TEMP,FAC1,FAC2,ERROR,ITERH)

C*****  CALCULATE ERROR EXACTLY (IE. CALCULATE NEW
C*****  COMPOSITION, IF NECESSARY, AND THEN ENTHALPY AT
C*****  GUESSED TEMPERATURE
C*****  CALCULATE COMPOSITION AT TEMP.

      CALL COMP(LCOSE,KINIT)

C*****  SKIP HLOSS CALCULATION FOR ADIABATIC CASE.

      QLOSS=0.0
      IF(NQHLS) 100,100,102
102 CONTINUE

C*****  EVALUATE STREAM PROPERTIES NEEDED FOR QLOSS CALC.

      CALL PROP(TWALL,YAVG,AVGMU,WALMU,RHO,TMASS,YTOT,CPAVG)

C*****  CALL PDROP TO CALCULATE PRESSURE DROP (AND TO SET
C*****  DIAMETER FOR SIMULATION CASE.)

      CALL PDROP(AVGMU,WALMU,RHO,TMASS,GT,ITERH)

C*****  CALCULATE TOTAL HEAT LOSS.

      CALL HLOSS (GT,CPAVG,TWALL,YTOT,YAVG)
100 CONTINUE

C*****  DEFINE ERROR AS REFERENCE ENTHALPY MINUS (ENTHALPY
C*****  AT THE GUESSED TEMP + HEAT LOSS).

      ERROR=ENTHR-ENTH-QLOSS
      IF(ITERH-3) 817,816,816
816 WRITE(IWRIT,5011) TEMP,ENTH,QLOSS,ERROR
817 CONTINUE

C*****  CONVERGENCE CHECK

      5 CRIT1=CRIT**(0.25+0.50*LOOSE)
      IF(ABS(ERROR/ENTHR)-CRIT1) 2,2,1

C*****  IF ERROR IS SMALL, INCREASE EQUILIBRIUM CRITERION.
C*****  IF THIS HAS BEEN DONE, TERMINATE

      2 IF(LOOSE) 3,3,4
      3 IF(ITERH-3) 11,10,10

```


SUBROUTINE TCALC ... (CONT'D)

```

11 LOOSE=1
   GO TO 1
10 LOOSE=1
   KINIT=0
   GO TO 5
   4 IF(IFNSH) 200,200,201
200 PRESS=PRESS-DELPC
   IFNSH=1
   GO TO 1
201 CONTINUE
   IF(ITEST-1) 801,800,800
800 IF(NOHL5) 301,301,302
301 WRITE(IWRIT,1001)
   GO TO 310
302 WRITE(IWRIT,3001)
   IF(IFLAG-1) 303,303,304
303 WRITE(IWRIT,3002)
   GO TO 310
304 WRITE(IWRIT,3003)
310 WRITE(IWRIT,9000)
   WRITE(IWRIT,4001) TEMP,PRESS,CRIT
   IF(NOHL5) 801,801,311
311 WRITE(IWRIT,8012) TDIAM,TNUMB,TLONG,DELPC,QLOSS
801 CONTINUE
   RETURN
1001 FORMAT( T34,'ITERATIVE ADIABATIC TEMPERATURE
$ CALCULATION')
3001 FORMAT(/ T32,'ITERATIVE NON-ADIABATIC TEMPERATURE
$ CALCULATION')
3002 FORMAT(T37,'TDIAM SPECIFIED, DELPC CALCULATED.')
3003 FORMAT(T37,'DELTP SPECIFIED, TDIAM CALCULATED.')
4001 FORMAT( T33,'FINAL CONVERGED TEMPERATURE IS ',F7.1,'
$ DEG. F'/T32,
1'PRESSURE (PSIA.) = ',F6.2,' (CRIT = ',E9.2,' )')
8012 FORMAT(/T43,'TUBE DIA. (IN.) = ',F6.2/T44,'NUMBER OF
$ TUBES = ',F5.
10/T42,'TUBE LENGTH (FT.) = ',F6.2/T41,'PRESSURE DROP
$ (PSI) = ',F6.
12/T35,'TOTAL HEAT LOSS (BTU.) = ',E15.7)
9000 FORMAT('0',T25,'*****
$*****
1*****'/ )
5010 FORMAT(1H0,'FEED TEMP. = ',F10.4,' DEG. F,
$ REFERENCE ENTHALPY
11S ',E15.7,' BTU.'/)
5011 FORMAT(1H0,'***** TEMP. = ',F10.4,' , ENTHALPY = '
$,E15.7,/'
10LOSS = ',E15.7,' ERROR = ',E15.7)
   END

```



```

C *****
C *
C *          SUBROUTINE GUESR
C *
C *  FUNCTIONS -
C *
C *  - ESTIMATE GENERATOR ROUTINE
C *  - USES THE SECANT METHOD TO PREDICT THE
C *    INDEPENDENT VARIABLE THAT WILL RESULT IN A
C *    ZERO ERROR FUNCTION
C *  - GIVEN AN INITIAL ESTIMATE AND A FACTOR FOR
C *    GENERATING A SECOND ESTIMATE FROM THE FIRST,
C *    PRODUCES THIRD AND SUBSEQUENT ESTIMATES FROM
C *    PREVIOUS ERRORS AND ESTIMATES
C *  - SAVES BEST PREVIOUS ESTIMATE
C *  - MUST BE GIVEN A CONVERGENCE ACCELERATOR
C *    (USUALLY 1 IF NO CONVERGENCE PROBLEM) --
C *    WILL EQUATE CONVERGENCE ACCELERATOR TO 1 AS
C *    CONVERGENCE PROCEEDS
C *
C *****

```

SUBROUTINE GUESR(GUESS,FAC1,FAC2,ERROR,ITERH)

```

C*****  THIS METHOD USES THE SECANT METHOD.  GUESS MUST
C*****  BE FOUND SUCH THAT THE ERROR BECOMES ZERO.  TWO
C*****  INITIAL GUESSES ARE REQUIRED TO INITIALIZE THE
C*****  METHOD.  THE FIRST IS SUPPLIED BY THE CALLING
C*****  PROGRAM ON THE FIRST CALL TO GUESR.  THE SECOND IS
C*****  GENERATED BY GUESR ON THE SECOND CALL.  SUBSEQUENT
C*****  GUESSES ARE DERIVED FROM THE LAST TWO GUESSES AND
C*****  ERRORS.

```

```

      ITERH=ITERH+1
      IF(ITERH-2) 100,102,103

```

```

C*****  STORE FIRST GUESS SUPPLIED BY CALLING ROUTINE.

```

```

      100 GUES1=GUESS
      RETURN

```

```

C*****  GENERATE SECOND GUESS FROM FIRST.  (STORE FIRST
C*****  ERROR AND SECOND GUESS).

```

```

      102 ERP1=ERROR
      GUESS=GUESS*FAC1
      GUES2=GUESS
      RETURN

```

```

C*****  THIRD OR GREATER GUESS.  GENERATE FROM LAST TWO
C*****  GUESSES AND ERRORS TO APPROX. GUESS FOR ZERO
C*****  ERROR.

```


SUBROUTINE GUESR ... (CONT'D)

103 GUESS=GUES1-FAC2*((GUES1-GUES2)*ERR1/(ERR1-ERROR))

C***** IF THIRD GUESS, SAVE BEST OF FIRST TWO GUESSES.

IF(ITERH-3) 104,104,105

104 IF(ABS(ERR1)-ABS(ERROR)) 106,106,105

105 GUES1=GUES2

ERR1=ERROR

106 GUES2=GUESS

IF(ITERH-4) 107,108,108

108 FAC2=1.0

107 RETURN

END


```

C *****
C *
C *          SUBROUTINE PROP
C *
C * FUNCTIONS -
C *
C * - STREAM PROPERTY EVALUATION ROUTINE
C * - CALCULATES STREAM PROPERTIES USING AN AVERAGE
C *   STREAM COMPOSITION AND AVERAGE TEMPERATURE
C * - EVALUATES AVERAGE COMPOSITION, AVERAGE AND WALL
C *   (SULPHUR DEW POINT) TEMPERATURES, GAS VISCOSITY,
C *   DENSITY, TOTAL STREAM MASS AND MOLES, AND
C *   AVERAGE STREAM HEAT CAPACITY
C *
C *****

```

```

      SUBROUTINE PROP(TWALL,YAVG,AVGMU,WALMU,RHO,TMASS,YTOT
      $,CPAVG)
      DIMENSION YAVG(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /DATA4/RMU(20),SMU(20),RADCT(20)
      COMMON /DATA5/IDH20,IDSUL(5),WTMOL(20),VMOLE(20)
      IF(ITEST-7) 811,810,810
      810 WRITE(IWRIT,9999)
      9999 FORMAT(1H0,' PROPERTY EVALUATION  ''PROP''
      $          '/')
      811 CONTINUE

```

```

C*****      CALCULATE MEAN TEMP. AS AVERAGE OF INLET (TFEED)
C*****      AND OUTLET (TEMP ) TEMPERATURES.

```

```

      TMEAN=(TFEED+TEMP )/2.0

```

```

C*****      CALCULATE MEAN COMPOSITION - AVERAGE OF TWO
C*****      COMPOSITIONS SATISFYING MASS BALANCES ALSO
C*****      SATISFYS IT.

```

```

      DO 40 I=1,NTOT
      40 YAVG(I)=(YCOMP(I)+YFEED(I))/2.0

```

```

C*****      CALCULATE TUBE WALL TEMP. (TWALL) =SULPHUR DEW PT.
C*****      TEMP.

```

```

      CALL DEWPT(TWALL,YAVG,PRESS,1)

```

```

C*****      CALCULATE STREAM VISCOSITY AT MEAN STREAM TEMP.
C*****      AND AT WALL TEMP. STREAM VISCOSITY IS WEIGHTED
C*****      (ROOT MOL. WT.) MEAN OF COMPONENT VISCOSITIES.
C*****      REF. - DERIVED FROM DATA IN PERRY'S CH. ENG.
C*****      HANDBOOK
C*****      DATA FORM- MU (CENTIPOISE) = RMU + SMU * T (DEG.F)

```


SUBROUTINE PROP ... (CONT'D)

```

SUM1=0.
SUM2=0.
SUM3=0.
DO 1 I=1,NGMS
YM=YAVG(I)*WTMOL(I)**0.5
SUM1=SUM1+YM
SUM2=SUM2+YM*(RMU(I)+SMU(I)*TMEAN)
1 SUM3=SUM3+YM*(RMU(I)+SMU(I)*TWALL)
AVGMU=SUM2/SUM1
WALMU=SUM3/SUM1

```

```

C*****      CALCULATE GAS STREAM MEAN DENSITY (RHO=LB/CU.FT)
C*****      USE IDEAL GAS LAW (PV=NRT) - FIRST CALCULATE
C*****      TOTAL MOLES AND TOTAL MASS

```

```

YTOT=0.
TMASS=0.
DO 2 I=1,NGMS
YTOT=YTOT+YAVG(I)
2 TMASS=TMASS+YAVG(I)*WTMOL(I)
RHO=TMASS*PRESS/(10.73*YTOT*(TMEAN+459.69))

```

```

C*****      CALCULATE STREAM MEAN HEAT CAPACITY AS MEAN OF
C*****      STREAM HEAT CAPACITIES AT TFEED AND TEMP.

```

```

CPAVG=(HFCAL(TFEED,YAVG,-1)+HFCAL(TEMP,YAVG,-1))/2.0
$*YTOT/TMASS
IF( ITEST-7) 801,800,800
800 WRITE(IWRIT,5000) TMEAN,YTOT,TMASS,AVGMU,WALMU,RHO
$,TWALL,CPAVG
801 CONTINUE
RETURN
5000 FORMAT(1H0,          'TMEAN = ',E15.7,2X,' YTOT = '
$,E15.7,2X,
1' TMASS = ',E15.7,/1X,'AVGMU = ',E15.7, 2X,'WALMU = '
$,E15.7,2X,
1' RHO = ',E15.7,/1X,'TDEWS = ',E15.7, 2X,'CPAVG = '
$,E15.7)
END

```



```

C *****
C *
C *          SUBROUTINE SUMER
C *
C *  FUNCTIONS -
C *
C *  -  STREAM SUMER ROUTINE
C *  -  DEPENDING UPON A FLAG, SUMS TOTAL MOLES AND
C *      MASS, TOTAL MOLES AND MASS OF ELEMENTAL
C *      SULPHUR OR, TOTAL ATOMS AND MASS OF (ATOMIC)
C *      SULPHUR IN A GIVEN STREAM
C *
C *****

```

```

      SUBROUTINE SUMEP (YDUMY, INDEX, IFLAG, TOTAL, TMASS)
      DIMENSION YDUMY(20)
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      COMMON /DATA1/FORMU(20,5), NATYP, IDATM(5)
      COMMON /DATA5/IDH2O, IDSUL(5), WTMOL(20), VMOLE(20)

```

```

C*****      IFLAG = 0 - SUM TOTAL MOLES AND MASS (ALL SPECIES)
C*****      1 - SUM TOTAL MOLES AND MASS (SULPHUR)
C*****      2 - SUM TOTAL ATOMS AND MASS (SULPHUR
C*****      ATOMS)

```

```

      TOTAL=0.0
      TMASS=0.0

```

```

C*****      DECIDE WHAT TO SUM.

```

```

      IF(IFLAG-1) 1,2,3

```

```

C*****      SUM ALL MOLECULAR SPECIES (TO INDEX INCLUSIVE).

```

```

      1 DO 10 I=1, INDEX
        TOTAL=TOTAL+YDUMY(I)
        TMASS=TMASS+YDUMY(I)*WTMOL(I)
      10 CONTINUE
      RETURN

```

```

C*****      SUM ALL PURE SULPHUR SPECIES (TO INDEX INCLUSIVE).

```

```

      2 DO 20 I=1,5
        ICNTS=IDSUL(I)
        IF(ICNTS) 20,20,15
      15 IF(ICNTS-INDEX) 16,16,20
      16 TOTAL=TOTAL+YDUMY(ICNTS)
        TMASS=TMASS+YDUMY(ICNTS)*WTMOL(ICNTS)
      20 CONTINUE
      RETURN

```

```

C*****      SUM TOTAL SULPHUR ATOMS IN ALL SPECIES

```


SUBROUTINE SUMER ... (CONT'D)

C***** (FROM 1 TO INDEX INCLUSIVE).

3 CONTINUE

C***** IDENTIFY SULPHUR COL. IN FORMU MATRIX.

```
      IROW=IDSUL(1)
      DO 25 J=1,NATYP
      IF(FORMU(IROW,J)-0.1) 25,25,26
25 CONTINUE
26 ICOL=J
      DO 30 I=1,INDEX
30 TOTAL=TOTAL+YDUMY(I)*FORMU(I,ICOL)
      TMASS=TOTAL*32.0
      RETURN
      END
```



```

C  ****
C  *
C  *          SUBROUTINE PRCNT
C  *
C  *  FUNCTIONS -
C  *
C  *  -  SULPHUR CONVERSION AND RECOVERY ROUTINE
C  *  -  CALCULATION BY-PASSED IF OUTPUT PRIORITY FLAG
C  *      IS OFF
C  *  -  STORES INPUT SULPHUR, FINDS REAL AND APPARENT
C  *      SULPHUR CONVERSION OR, FINDS TOTAL PLANT
C  *      SULPHUR RECOVERY, DEPENDING UPON A FLAG
C  *  -  FOR LAST CASE, ALSO COMPLETES PLANT MASS AND
C  *      ENERGY BALANCES
C  *
C  ****

```

```

SUBROUTINE PRCNT(IFLAG)
  DIMENSION NAME(5),ATIN(5),ATOUT(5),YDUMMY(20)
  COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
  COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,FNTH
  COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)
  COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
  DATA NAME/'S ','O ','C ','H ','N '/
  IF(ITEST-1) 900,100,100
100 CONTINUE
  IF(IFLAG-2) 1,2,3
  1 CALL SUMER(YFEED,NTOT,1,TOTS,TSM1)
  CALL SUMER(YFEED,NTOT,2,TOTS,TSM2)
  IF(IFLAG-3) 900,2,2
  2 CALL SUMER(YCOMP,NTOT,1,TOTS,TSM3)
  CONV1=TSM3/TSM2*100.0
  CONV2=(TSM3-TSM1)/(TSM2-TSM1)*100.
  WRITE(IWRIT,1000) CONV1
  IF(ABS(CONV1-CONV2)-0.1) 11,11,10
10 WRITE(IWRIT,1001) CONV2
11 WRITE(IWRIT,9000)
  GO TO 900
  3 CONTINUE
  ENIN=0.0
  ENOUT=0.0
  DO 40 I=1,NTOT
  YFEED(I)=0.0
40 YCOMP(I)=0.0
  DO 50 I=1,50
  IF(INFO(I,1)) 50,50,51
51 IF(INFO(I,5)) 50,52,50
52 IF(INFO(I,2)) 54,53,54
53 CALL SUTIL(I,1,YDUMMY,TEMP,PRESS)
  DO 60 J=1,NTOT
60 YFEED(J)=YFEED(J)+YDUMMY(J)
  FNIN=ENIN+HFCAL(TEMP,YDUMMY,0)

```


SUBROUTINE PRCNT ... (CONT'D)

```

      GO TO 50
54  IF(INFO(I,3)) 50,55,50
55  CALL SUTIL(I,1,YDUMY,TEMP,PRESS)
      DO 61 J=1,NTOT
61  YCOMP(J)=YCOMP(J)+YDUMY(J)
      ENOUT=ENOUT+HFCAL(TEMP,YDUMY,0)
50  CONTINUE
      WRITE(IWRIT,2000)
      WRITE(IWRIT,9000)
      WRITE(IWPIT,2020)
      ATOTL=0.0
      ERROR=0.0
      DO 68 I=1,5
        ATIN(I)=0.0
        ATOUT(I)=0.0
68  CONTINUE
      DO 70 J=1,5
        ICOL=IDATM(J)
        DO 69 I=1,NTOT
          ATIN(ICOL)=ATIN(ICOL)+FORMU(I,ICOL)*YFEED(I)
          ATOUT(ICOL)=ATOUT(ICOL)+FORMU(I,ICOL)*YCOMP(I)
69  CONTINUE
          ATOUT(ICOL)=(ATIN(ICOL)-ATOUT(ICOL))/ATIN(ICOL)*100.0
          WRITE(IWRIT,2001) NAME(J),ATIN(ICOL),ATOUT(ICOL)
          ATOTL=ATOTL+ATIN(ICOL)
          ERROR=ERROR+ATIN(ICOL)*ATOUT(ICOL)
70  CONTINUE
          ERROR=ERROR/ATOTL
          WRITE(IWRIT,2002) ATOTL,ERROR
          WRITE(IWRIT,9000)
          DIFF=ENIN-ENOUT
          WRITE(IWRIT,2003) ENIN,ENOUT,DIFF
          WRITE(IWRIT,9000)
          WRITE(IWRIT,1002)
          GO TO 1
900  RETURN
1000  FORMAT(//T40'PERCENT OF TOTAL INLET SULPHUR'/T39'OUT
      $ AS ELEMENTAL
      1SULPHUR = 'F6.2)
1001  FORMAT(//T37'PERCENT OF NON-ELEMENTAL INLET SULPHUR'
      $ /T39'OUT AS
      1 ELEMENTAL SULPHUR = 'F6.2)
1002  FORMAT('0'T40'OVERALL PLANT SULPHUR RECOVERY')
2000  FORMAT('1'/////T36'OVERALL PLANT MASS AND ENERGY
      $ BALANCE')
2020  FORMAT(T41'ATOM AND TOTAL MASS BALANCES'/
      $/T37'ATOM'T51'ATOM'T65'PE
      1PCENT'/T37'TYPE'T51'TOTAL'T66'ERROR'/)
2001  FORMAT('0'T39,A1,7X,E13.6,5X,F7.5)
2002  FORMAT('0'T37'TOTAL'5X,E13.6,5X,F7.5)

```


SUBROUTINE PRONT ... (CONT'D)

```
2003 FORMAT('O'T48'ENERGY BALANCE'//T38'(ENTHALPY IS
$ RELATIVE AND IN BT
10.)'//T41'ENTHALPY IN = 'E13.6//T41'ENTHALPY OUT =
$ 'E13.6//T41'DI
1FFERENCE = 'E13.6//T34'DIFFERENCE SHOULD BE TOTAL
$ PLANT HEAT LOA
1D')
9000 FORMAT('O',T25,'*****')
$*****
1*****')
END
```



```

C *****
C *
C *          SUBROUTINE STEAM
C *
C *  FUNCTIONS -
C *
C *  - STEAM PRODUCTION CALCULATION ROUTINE
C *  - FINDS CORRECTED LATENT HEAT OF STEAM AND
C *    STEAM PRODUCTION (LBS, AND MOLES) FOR A GIVEN
C *    DUTY, FEEDWATER STREAM AND STEAM TEMPERATURE
C *  - STORES RELEVANT STEAM FEED AND PRODUCT STREAMS
C *    IF PRESENT
C *
C *****

      SUBROUTINE STEAM(DUTY,TSTEM,PSTEM,NSTMS,NSTMP,IPAR)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)

C*****      STORE STEAM PRESSURE IN EQUIP VECTOR.

      IVAL=ILOC+IPAR
      EQUIP(IVAL)=SIGN(PSTEM,EQUIP(IVAL))
      COREC=0.0

C*****      IF STEAM FEED-WATER STREAM EXISTS, CHECK ITS TEMP.

      IF(NSTMS) 100,100,10
10  TSIN=ABS(STREM(NSTMS,21))
      IF(TSIN) 12,12,11

C*****      IF TEMPERATURE (FEED-WATER) SPECIFIED, CALCULATE
C*****      LATENT HEAT CORRECTION TO COMPENSATE FOR HEATING
C*****      (COOLING) TO THE SATURATION TEMP. CORRESPONDING TO
C*****      GIVEN PRESS. (ASSUME 1.0 BTU./LB.DEG.F)

11  COREC=TSTEM-TSIN
      GO TO 100

C*****      IF FEED-WATER TEMP. NOT GIVEN, SET TO SAT. TEMP.

12  STREM(NSTMS,21)=TSTEM

C*****      CALCULATE LATENT HEAT OF FEED-WATER AT SAT. TEMP.
C*****      THEN CORRECT THIS TO EXISTING CONDITIONS.

100 DELHV=EXP(7.0095+0.3542*ALOG(1.0-TSTEM/705.4))
      CDELH=DELHV+COREC

C*****      CALCULATE STEAM PRODUCTION.

```


SUBROUTINE STEAM ... (CONT'D)

PROD=DUTY/CDELH

C***** IF FEED-WATER STREAM EXISTS, SET PRESSURE AND FLOW

IF(NSTMS) 21,21,20

20 STREM(NSTMS,22)=SIGN(PSTEM,EQUIP(IVAL))

STREM(NSTMS,IDH20)=PROD/WTMOL(IDH20)

C***** IF STEAM PROD. STREAM EXISTS, SET PRESS,TEMP. AND
C***** FLOW.

21 IF(NSTMP) 23,23,22

22 STREM(NSTMP,22)=SIGN(PSTEM,EQUIP(IVAL))

STREM(NSTMP,21)=TSTEM

STREM(NSTMP,IDH20)=PROD/WTMOL(IDH20)

C***** PRINT RESULTS IF REQUIRED.

23 IF(ITEST-1) 801,800,800

800 WRITE(IWRIT,7000) DUTY,TSTEM,PSTEM,DELHV,CORREC,PROD
WRITE(IWRIT,9000)

801 CONTINUE
RETURN

7000 FORMAT(///T25'EQUIP. HEAT DUTY (BTU/HR) IS',T70,E15.7/

\$/T25'STEAM

1TEMP. (DEG,F.) = ',T71,F7.1/T32'PRESS. (PSIA) ='T70

\$,F8.3/T32'LATEN

1T HEAT (BTU/LB) = ',T71,F7.1,/T32,'L.H. CORRECTION

\$ ='T71,F7.1/T32,

1'PRODUCTION (LB/HR) ='T63,F15.7)

9000 FORMAT('0',T25,'*****')

\$*****

1*****' /)

END


```

C *****
C *
C *          SUBROUTINE AIRFD
C *
C *  FUNCTIONS -
C *
C *  -  COMBUSTION AIR REQUIREMENT ROUTINE
C *  -  FINDS AIR STREAM (NITROGEN, OXYGEN AND WATER)
C *      REQUIRED TO COMPLETE A SPECIFIED COMBUSTION
C *  -  REQUIRES FRACTION OF SULPHUR TO BE BURNED,
C *      EXCESS OR DEFICIENT AIR COEFFICIENT AND AIR
C *      RELATIVE HUMIDITY, PRESSURE AND TEMPERATURE
C *      SPECIFICATIONS
C *  -  STORES AIR STREAM SEPARATELY -- ALSO ADDS AIR
C *      TO GIVEN STREAM TO BE COMBUSTED AND FINDS
C *      RESULTING COMBINED TEMPERATURE
C *
C *****

```

```

      SUBROUTINE AIRFD (YCOMP,TEMP,SPEC1,SPEC2,RELHY,YAIR
5,TAIR,PAIR)
      DIMENSION SUMS(4),YAIR(20),YCOMP(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)
      COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)
      DATA IDFY/0/
      IF(IDFY) 1,1,2
1  ICHEK=0
      DO 10 I=1,NGMS
      INDIC=IDATM(2)
      IF(FORMU(I,INDIC)-0.01) 5,5,50
5  INDIC=IDATM(5)
      IF(FORMU(I,INDIC)-0.01) 10,10,50
50 DO 60 J=1,NATYP
      IF(J-INDIC) 55,60,55
55 IF(FORMU(I,J)-0.01) 60,60,10
60 CONTINUE
      IF(INDIC-IDATM(2)) 62,61,62
61 NO2=I
      ICHEK=ICHEK+1
      GO TO 10
62 NN2=I
      ICHEK=ICHEK+1
10 CONTINUE
      IDFY=1
      IF(ICHEK-2) 500,2,500
500 WRITE(IWRIT,5000)
2  CONTINUE
      DO 99 J=1,4
99 SUMS(J)=0.0
      DO 100 J=1,4
      NCOL=IDATM(J)

```


SUBROUTINE AIRED ... (CONT'D)

```

      DO 100 I=1,NTOT
      SUMS(J)=SUMS(J)+FORMU(I,NCOL)*YCOMP(I)
100  CONTINUE
      DO 200 I=1,NTOT
200  YAIR(I)=0.0
      YAIR(N02)=SPEC1*0.5*(SUMS(1)*2.*SPEC2+SUMS(3)*2.
1  +(SUMS(4)-2.*SUMS(1)*(1.-SPEC2))*0.5-SUMS(2))
      YAIR(NN2)=YAIR(N02)*79./21.
      CALL VPRES(VPH20,DUMY,TAIR,0)
      VPH20=VPH20*14.696*RELHY/100.
      YAIR(IDH20)=(VPH20*(YAIR(N02)+YAIR(NN2))
1  /(PAIR-VPH20))
      ENTHR=HFCAL(TEMP,YCOMP,0)+HFCAL(TAIR,YAIR,0)
      DO 201 I=1,NTOT
201  YCOMP(I)=YCOMP(I)+YAIR(I)
      CALL FINDT(YCOMP,TEMP,ENTHR)
      RETURN
5000 FORMAT('OERROR W.R.T. PRESENCE OF O2 AND/OR N2
$ SPECIES')
      END

```



```

C *****
C *
C *          SUBROUTINE BKBOX
C *
C *  FUNCTIONS -
C *
C *  -  (BLACK BOX) DUMMY EQUIPMENT MODULE (ITYPE=10)
C *  -  SOLE EQUIPMENT PARAMETER IS TCTOF (EQUILIBRIUM
C *      CUTOFF TEMPERATURE) -- ASSUMED AS -1 IF NOT
C *      GIVEN (I.F. SULPHUR SHIFT ON GIVEN STREAM)
C *  -  ALTERS INLET TEMPERATURE AND PRESSURE TO THE
C *      OUTLET CONDITIONS (TEMPERATURE AND PRESSURE)
C *      SPECIFIED AS *STREAM SPECIFICATION* DATA. IF
C *      LATTER IS NOT GIVEN, OUTPUT EQUATED TO INPUT
C *  -  IF OUTPUT CONDITIONS (T AND P) GIVEN, COMPLETES
C *      COMPOSITION CALCULATION (DEPENDING UPON TCTOF)
C *      AT SPECIFIED OUTPUT CONDITIONS AND STORES
C *      OUTPUT MOLE NUMBERS.  ENTHALPY DIFFERENCE
C *      BETWEEN INPUT AND OUTPUT IS CALCULATED.
C *
C *****

```

```

      SUBROUTINE BKBOX
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      COMMON /GEN2/TEMP, TFEED, YCOMP(20), YFEED(20), PRESS, ENTH
      COMMON /STOR1/EQUIP(300), ILOC, NMBEQ, STREM(50, 22)
      $, NSIN(5), NSOUT(5)
      COMMON /BURN1/TCTOF, TBURN, IMUFF, NLGTH, NDIAM, NRTIM
      $, NHRLS, NBURN
      WRITE(IWRIT, 6000) NMBEQ
      NSTRM=0
      CALL SUTIL(NSTRM, 0, YFEED, TFEED, PRESS)
      CALL PRNTS(-1)
      TCTOF=SETVU(-EQUIP(ILOC+1), -1.0)
      PFEED=PRESS
      HREF=HFCAL(TFEED, YCOMP, 0)
      NEXIT=NSOUT(1)
      CALL SUTIL(NEXIT, 1, YCOMP, TEMP, PRESS)
      PRESS=SETVU(PRESS, PFEED)
      TEMP=SETVU(TEMP, TFEED)
      DO 1 I=1, NTOT
1  YCOMP(I)=YFEED(I)
      LOOSE=1
      KINIT=1
      CALL COMP(LOOSE, KINIT)
      CALL SUTIL(NEXIT, 2, YCOMP, TEMP, PRESS)
      HDIFF=HFCAL(TEMP, YCOMP, 0)-HREF
      IF(ITEST-1) 301, 800, 800
800 WRITE(IWRIT, 1000) TFEED, TEMP, HDIFF
      WRITE(IWRIT, 9000)
      CALL PRNTS(NEXIT)
801 CONTINUE

```


SUBROUTINE BKBOX ...(CONT'D)

```
      RETURN
1000  FORMAT(T31'TEMPERATURE CHANGED FROM 'F6.1' TO 'F6.1'
      $ DEG.F.'//
      1T32'(ENTHALPY DIFFERENCE IS 'E13.6' BTU/HR.)')
6000  FORMAT(T50'BLACK BOX'/T45'EQUIPMENT NUMBER 'I3)
9000  FORMAT('0',T25,'*****
      $*****
      1 *****')
      END
```



```

C *****
C *
C *          SUBROUTINE COMP
C *
C *  FUNCTIONS -
C *
C *  - PRIMARY COMPOSITION CALCULATION ROUTINE
C *  - DECIDES WHETHER TO DO COMPLETE EQUILIBRIUM
C *    CALCULATION AT GIVEN TEMPERATURE, EQUILIBRIUM
C *    AT CUTOFF TEMPERATURE, SULPHUR SHIFT ON
C *    CUTOFF COMPOSITION OR SULPHUR SHIFT ON
C *    GIVEN COMPOSITION
C *  - STORES CUTOFF EQUILIBRIUM COMPOSITION SO THAT
C *    IT NEED BE CALCULATED ONLY ONCE
C *
C *****

```

```

      SUBROUTINE COMP(LOOSE,KINIT)
      DIMENSION BSTOR(5),YCTOF(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)
      COMMON /BURN1/TCTOF,TBURN,IMUFF,NLGTH,NDIAM,NRTIM
      $,NHRLS,NBURN
      NSTOR=NGMS
      CSTOR=TCTOF
      CALL FAKER(NGMS,TCTOF,TEMP)
      CRITS=CRIT
      IF(LOOSE)100,100,101
100 CRIT=CRIT**0.25
101 CONTINUE

```

```

C*****      CHECK TO SEE IF TEMPERATURE (TEMP ) IS BELOW
C*****      EQUILIBRIUM CUT-OFF TEMPERATURE (TCTOF). IF IT
C*****      IS BELOW, USE STREAM COMPOSITION AT TCTOF.

```

```

      IF(ITEST-4) 803,800,800
800 IF(TEMP -TCTOF) 801,801,802
801 WRITE(IWRIT,5000) TEMP ,TCTOF
      GO TO 803
802 WRITE(IWRIT,5001) TEMP ,TCTOF
803 CONTINUE
      IF(TEMP -TCTOF) 1,1,3

```

```

C*****      CHECK IF EQUIL. AT THIS CUTOFF TEMP. HAS BEEN
C*****      PREVIOUSLY CALCULATED. IF NOT, CALCULATE IT NOW

```

```

1 IF(ABS((TSTOR-TCTOF)/TCTOF)-1.0E-4) 2,2,6

```

```

C*****      CHECK IF PREVIOUS CALCULATIONS WERE FOR AN
C*****      IDENTICAL STREAM - USE ATOM TOTALS (B'S) FOR
C*****      STREAM COMPARISON - IF STREAM DIFFERENT,

```


SUBROUTINE COMP ... (CONT'D)

C***** CALCULATE NEW EQUIL. COMP. AT TCTOF

```

2 DO 4 J=1,NATYP
  TOT=0.
  DO 3 I=1,NGMS
3  TOT=TOT+FORMU(I,J)*YCOMP(I)
  IF(ABS((TOT-BSTOR(J))/TOT)-1.0E-4) 4,4,6
4  CONTINUE

```

C***** EQUIL. AT THIS EQUIL. CUT-OFF TEMP. FOR AN
 C***** IDENTICAL STREAM HAS BEEN PREVIOUSLY CALCULATED,
 C***** SO EQUATE TO PREVIOUS RESULTS

```

  IF(ITEST-4) 809,808,808
808 WRITE(IWRIT,5004)
809 CONTINUE
  DO 5 I=1,NGMS
5  YCOMP(I)=YCTOF(I)
  GO TO 99

```

C***** CALCULATE STREAM COMPOSITION AT TCTOF

```

6 IF(ITEST-4) 807,806,806
806 WRITE(IWRIT,5003) TCTOF
807 CONTINUE

```

C***** CALCULATE RIGOROUSLY (ONLY DONE ONCE)

```

  IF(LOOSE) 20,20,21
20 CRIT=CRITS
21 CALL MINFE(PRESS,TCTOF,YCOMP,KINIT)
  TSTOR=TCTOF

```

C***** STORE THIS EQUILIBRIUM COMPOSITION AND ATOM TOTALS
 C***** FOR FUTURE USE.

```

  DO 10 J=1,NATYP
10  BSTOR(J)=0.0
  DO 7 I=1,NGMS
  YCTOF(I)=YCOMP(I)
  DO 7 J=1,NATYP
7  BSTOR(J)=BSTOR(J)+YCOMP(I)*FORMU(I,J)
99 CALL SHIFT(KINIT,NTOT)
  DO 12 I=1,NGMS
12 YCTOF(I)=YCOMP(I)
  GO TO 9

```

C***** IF TCTOF IS NEGATIVE, JUST DO SULPHUR SHIFT ON
 C***** GIVEN STREAM.

SUBROUTINE COMP ... (CONT'D)

8 IF(TCTOF+1E-10)99,98,98

C***** CALCULATE EQUILIBRIUM COMPOSITION AT SPECIFIED
C***** TEMPERATURE

98 IF(ITEST-4) 805,804,804
804 WRITE(IWRIT,5002) TEMP
805 CONTINUE
CALL MINFE(PRESS,TEMP ,YCOMP,KINIT)

C***** CALCULATE ENTHALPY OF STREAM AT SPECIFIED
C***** TEMPERATURE

9 ENTH=HFCAL(TEMP ,YCOMP,0)
CRIT=CRITS
NGMS=NSTOR
TCTOF=CSTOR
RETURN
5000 FORMAT(1H0,'TEMP. (' ,F10.4,' DEG.F), IS BELOW TCTOF
\$ ('F10.4,')')
5001 FORMAT(1H0,'TEMP.(' ,F10.4,' DEG.F), IS ABOVE TCTOF
\$ ('F10.4,')')
5002 FORMAT(1H , 'CALCULATE COMPOSITION AT ' ,F10.4,' DEG.
\$ F')
5003 FORMAT(1H , 'CALCULATE COMPOSITION AT CUTOFF TEMP. ('
\$,F10.4,')')
5004 FORMAT(1H , ' COMP. AT CUTOFF HAS BEEN CALCULATED, USE
\$ PREVIOUS RES
1ULTS')
END


```

C  ****
C  *
C  *          SUBROUTINE SHIFT
C  *
C  *  FUNCTIONS -
C  *
C  *  -  SULPHUR SHIFT ROUTINE
C  *  -  EXTRACTS SULPHUR VAPOR SPECIES (AND OPTIONALLY
C  *      LIQUID SULPHUR) FROM GIVEN STREAM --
C  *      INTRODUCES THEM INTO A DUMMY STREAM
C  *  -  CALCULATES EQUILIBRIUM COMPOSITION FOR THIS
C  *      DUMMY STREAM AT GIVEN TEMPERATURE AND EXISTING
C  *      SULPHUR PARTIAL PRESSURE.
C  *  -  ITERATES ON COMPOSITION CALCULATION UNTIL
C  *      SULPHUR PARTIAL PRESSURE CONVERGES
C  *  -  SKIPS CALCULATION IF NO SULPHUR IN GIVEN
C  *      STREAM
C  *
C  ****

```

```

      SUBROUTINE SHIFT(KINIT,NIND)
      DIMENSION YDUMMY(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)
      KSTOR=KINIT
      IF(ITEST-4) 801,800,800
800  WRITE(IWRIT,1000) (IDSUL(I),I=1,5)
801  CONTINUE
      YTOT=0.0
      STOT=0.0
      DO 100 I=1,NGMS
      YTOT=YTOT+YCOMP(I)
100  YDUMMY(I)=0.0
      DO 1 I=1,5
      K=I
      II=IDSUL(I)
      IF(II) 9,9,2
9  K=I-1
      GO TO 12
2  YDUMMY(II)=YCOMP(II)
      IF(II-NGMS)3,3,4
3  STOT=STOT+YDUMMY(II)
      GO TO 1
4  IF(II-NIND) 5,5,9
5  ISUB=IDSUL(1)
      STOT=STOT-YDUMMY(ISUB)
      YDUMMY(ISUB)=YDUMMY(ISUB)+YCOMP(II)*WTMOL(II)
      $/WTMOL(ISUB)
      STOT=STOT+YDUMMY(ISUB)
      YDUMMY(II)=0.0
1  YCOMP(II)=0.0

```


SUBROUTINE SHIFT ... (CONT'D)

```
12 CONTINUE
   IF (STOT-1.E-3) 50,50,11
11  PARTP=PRESS*STOT/YTOT
51  CALL MINFE(PARTP,TEMP,YDUMY,KINIT)
   DO 200 I=1,K
   II=IDSUL(I)
200  YCOMP(II)=YDUMY(II)
   CALL SUMER(YCOMP,NGMS,1,STOT,DUMY)
   CALL SUMER(YCOMP,NGMS,0,YTOT,DUMY)
   POLD=PARTP
   KINIT=0
   PARTP=PRESS*STOT/YTOT
   IF (ABS(PARTP-POLD)/POLD-CRIT**0.5) 50,50,51
50  CONTINUE
   KINIT=KSTOR
   RETURN
1000 FORMAT('0  SULPHUR SHIFT CALCULATION, COMPONENTS - '
$,5I3)
   END
```



```

C *****
C *
C *          SUBROUTINE MINFE
C *
C *  FUNCTIONS -
C *
C *  - FREE ENERGY MINIMIZATION ROUTINE
C *  - INITIALIZES THE EQUILIBRIUM CALCULATIONS
C *  - FOR EACH ITERATION, SETS UP THE MATRIX FOR
C *    DETERMINING THE LAGRANGIAN MULTIPLIERS
C *  - CALCULATES THE PREDICTED MOLE NUMBER CORRECTIONS
C *
C *****

```

```

      SUBROUTINE MINFE(PRESS,TDEGF,YDUMY,KINIT)
      DOUBLE PRECISION Z,R,S,YBAR,SUM,F,B,RATIO,ADD,YCOMP
      DIMENSION B(5),YCOMP(20),F(20),STORE(20),Z(6,6),R(6)
      $,S(6),ADD(20)
      DIMENSION INDB(5),IPOS(20),YDUMY(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)
      IF(IDBUG(12)-1) 801,800,800
      800 WRITE(IWRIT,5000)
      801 CONTINUE
      DO 200 I=1,NGMS
      200 YCOMP(I)=DBLE(YDUMY(I))

```

```

C*****      CALL INIT TO INITIALIZE THE FREE ENERGY
C*****      MINIMIZATION AND TO GENERATE AN INITIAL POSITIVE
C*****      SET OF MOLE NUMBERS IF NECESSARY
C*****      IPOS,STORE,NATPR AND B ARE DEFINED BY INIT

```

```

      CALL INIT(PRESS,TDEGF,YCOMP,B,STORE,INDB,IPOS,NATPR
      $,KINIT)
      MPI=NATPR+1

```

```

C*****      ITER - ITERATION COUNTER

```

```

      ITER=0
      101 CONTINUE

```

```

C*****      HERE TO 3 - SET UP MATRIX EQUATION TO FIND
C*****      LAGRANGIAN MULTIPLIERS - THESE ARE USED TO
C*****      GENERATE A NEW SET OF MOLE NUMBERS. ONLY ATOM
C*****      TYPES PRESENT AND MOLECULAR SPECIES POSSIBLE (AS
C*****      DETERMINED BY INIT) ARE CONSIDERED.

```

```

      ITER=ITER+1

```

```

C*****      HERE TO 1 - SUM MOLE NUMBERS

```

```

      YBAR=0

```


SUBROUTINE MINFE ... (CONT'D)

```

DO 1 I=1,NGMS
YBAR=YBAR+YCOMP(I)
1 CONTINUE

```

C***** HERE TO 2 - CALCULATE FREE ENERGY FUNCTIONS

```

SUM=0
DO 2 I=1,NGMS
F(I)=0.0
IF(YCOMP(I)) 2,2,10
10 CONTINUE
F(I)=YCOMP(I)*(STORE(I)+DLOG(YCOMP(I)/YBAR))
SUM=SUM+F(I)
2 CONTINUE
R(MP1)=SUM
DO 3 J=1,NATPR
IND=INDB(J)
Z(J,MP1)=B(IND)
Z(MP1,J)=B(IND)
SUM=0
DO 5 I=1,NGMS
SUM=SUM+FORMU(I,IND)*F(I)
5 CONTINUE
R(J)=SUM
DO 3 K=1,NATPR
IND1=INDB(K)
SUM=0
DO 4 I=1,NGMS
SUM=SUM+FORMU(I,IND)*FORMU(I,IND1)*YCOMP(I)
4 CONTINUE
Z(J,K)=SUM
Z(K,J)=SUM
3 CONTINUE
Z(MP1,MP1)=0
IF(IDBUG(12)-10) 806,804,804
804 WRITE(IWRIT,5002)
DO 805 I=1,MP1
805 WRITE(IWRIT,5003) (Z(I,J),J=1,MP1),R(I)
806 CONTINUE

```

C***** CALL GAUSS TO SOLVE THE CONSTRUCTED MATRIX
C***** EQUATION FOR THE LAGRANGIAN MULTIPLIERS
C***** Z - SQUARE MATRIX , DIMENSION MP1
C***** R - RIGHT HAND SIDE
C***** S - SOLUTION VECTOR

```

CALL GAUSS (Z,R,MP1,S)
IF(IDBUG(12)-10) 808,807,807
807 WRITE(IWRIT,5004) (S(I),I=1,MP1)
808 CONTINUE

```


SUBROUTINE MINFE ... (CONT'D)

```

C***** HERE TO 6 - CALCULATE THE CORRECTIONS TO THE
C***** MOLE NUMBERS (ADD) WHICH WILL RESULT IN A BETTER
C***** APPROXIMATION TO THE EQUILIBRIUM COMPOSITION
C***** (MINIMUM SYSTEM FREE ENERGY)

```

```

      RATIO=S(MP1)+1.0
      DO 6 I=1,NGMS
      SUM=0
      DO 7 J=1,NATPR
      IND=INDB(J)
      SUM=SUM+S(J)*FORMU(I,IND)
7 CONTINUE
      ADD(I)=(-F(I)+(RATIO+SUM)*YCOMP(I))-YCOMP(I)
6 CONTINUE
      IF(IDBUG(12)-8) 803,802,802
802 WRITE(IWRIT,5001) (ADD(I),I=1,NGMS)
803 CONTINUE

```

```

C***** CALL YMODY TO PREVENT NEGATIVE MOLE NUMBERS OR
C***** PREMATURE ZEROING OF MOLE NUMBERS AND TO CHECK FOR
C***** CONVERGENCE

```

```

      CALL YMODY(YCOMP,ADD,ICNT,ITER,TDEGF,PRESS,IPOS)

```

```

C***** IF CONVERGED (ICNT=NGMS), TERMINATE, OTHERWISE
C***** ITERATE

```

```

      IF(ICNT-NGMS) 101,100,100
100 DO 201 I=1,NGMS
201 YDUMY(I)=SNGL(YCOMP(I))
      RETURN
5000 FORMAT(1H0,' EQUILIBRIUM COMPOSITION CALCULATION' )
5001 FORMAT(1H0,'CORRECTIONS ARE - '/(5E15.7))
5002 FORMAT(1H0,'AUGMENTED MATRIX FOR CALCULATION OF
      $ LAGRANGIAN MULTIPL
      1IERS IS - ' )
5003 FORMAT(1H ,7E15.7)
5004 FORMAT(1H ,/' SOLUTION IS - '/6E15.7 )
      END

```



```

C *****
C *
C *          SUBROUTINE INIT
C *
C * FUNCTIONS -
C *
C * - EQUILIBRIUM INITIALIZATION ROUTINE
C * - DEPENDING UPON A FLAG, GENERATES A POSITIVE
C *   SET OF MOLE NUMBERS OR SKIPS THIS GENERATION
C * - CALCULATES THE ATOM TOTALS, AND FREE ENERGY
C *   FUNCTIONS, AND FLAGS ALL IMPOSSIBLE SPECIES SO
C *   THEY WILL BE IGNORED DURING THE MINIMIZATION
C *
C *****

```

```

SUBROUTINE INIT(PRESS,TDEGF,YCOMP,B,STORE,INDB,IPOS
$,NATPR,KINIT)

```

```

DOUBLE PRECISION YCOMP,B

```

```

DIMENSION B(5),YCOMP(20),STORE(20),INDB(5),IPCS(20)

```

```

COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT

```

```

COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)

```

```

C*****      NGMS  - TOTAL NUMBER OF MOLECULAR SPECIES LISTED
C*****      (CORRESPONDS TO ROWS OF MATRIX FORMU)
C*****      IPOS(I) = 1  IF ITH MOLECULAR SPECIE PHYSICALLY
C*****      FEASIBLE. (IE. ALL CONSTITUENT ATOMS
C*****      ARE PRESENT IN THE STREAM
C*****      = 0  IF ITH SPECIE IS NOT FEASIBLE
C*****      B(J)  - JTH ATOM TOTAL IN STREAM
C*****      NATYP  - TOTAL NUMBER OF ATOM TYPES LISTED
C*****      (CORRESPONDS TO COLUMNS OF MATRIX FORMU)
C*****      NATPR  - TOTAL NUMBER OF ATOM TYPES PRESENT
C*****      -INDB  - ITH ELEMENT OF INDB CORRESPONDS TO THE
C*****      -      COLUMN OF THE ITH NON-ZERO ATOM TYPE
C*****      -      (IN MATRIX FORMU)
C*****

```

```

      IF(IDBUG(12)-4) 801,800,800
800 WRITE(IWRIT,5000) (YCOMP(I),I=1,NGMS)
      IFLAG=0
801 CONTINUE

```

```

C*****      -INITIALIZE IPOS ELEMENTS TO 1, AND CALCULATE FREE
C*****      ENERGY -FUNCTIONS (F/RT + LN P)

```

```

      DO 1 I=1,NGMS
      IPOS(I)=1
      STORE(I)=HFCAL(TDEGF,YCOMP,I)+ALOG(PRESS/14.696)
1 CONTINUE
      IF(IDBUG(12)-9) 809,808,808
808 WRITE(IWRIT,5005) (STORE(I),I=1,NGMS)
809 CONTINUE

```


SUBROUTINE INIT ... (CONT'D)

```
IND=1
NATPR=NATYP
```

```
C***** HERE TO 3 - CALCULATE ATOM TOTALS, AND SET IPOS
C***** AND INDB VECTOPS
```

```
DO 3 J=1,NATYP
```

```
C***** CALCULATE ATOM TOTAL (B(J))
```

```
B(J)=0.0
DO 4 I=1,NGMS
  B(J)=B(J)+FORMU(I,J)*YCOMP(I)
4 CONTINUE
  IF(B(J)-1.0E-30) 40,40,43
```

```
C***** -IF ATOM TOTAL IS ZERO, SET IPOS ENTRIES FOR ALL
C***** MOLECULAR -SPECIES CONTAINING THAT ATOM TYPE TO
C***** ZERO, AND DECREMENT MM.
```

```
40 DO 41 I=1,NGMS
  IF(FORMU(I,J)-1.0E-30) 41,41,42
42 IPOS(I)=0
41 CONTINUE
  NATPR=NATPR-1
  GO TO 3
```

```
C***** -IF ATOM TOTAL NON-ZERO, STORE MATRIX COLUMN
C***** NUMBER IN INDB
```

```
43 INDB(IND)=J
  IND=IND+1
3 CONTINUE
  IF(IDBUG(12)-5) 803,802,802
802 WRITE(IWRIT,5001) (IPOS(I),I=1,NGMS)
  WRITE(IWRIT,5002) (B(I),I=1,NATYP)
803 CONTINUE
```

```
C***** HERE TO 5 - GENERATE AN INITIAL POSSITIVE SET OF
C***** MOLE NUMBERS , (FOR THE FREE ENERGY MINIMIZATION )
C***** , IF ONE DOES NOT ALREADY EXIST. EQUATE POSSIBLE
C***** MOLECULAR SPECIES (IPOS=1) WHICH ARE ZERO TO AN
C***** ARBITRARILY SMALL AMOUNT. THIS INTRODUCES A SMALL
C***** ERROR INTO THE MASS BALANCES, BUT IS NECESSARY TO
C***** FACILITATE A VALID EQUILIBRIUM COMPOSITION
C***** CALCULATION.
C***** IF KINIT=0 , SKIP THIS SECTION.
```

```
IF(KINIT) 900,900,100
```


SUBROUTINE INIT ... (CONT'D)

```
100 DO 5 I=1,NGMS
```

```
C***** CHECK IF MOLE NUMBER IS ZERO
```

```
IF(YCCMP(I)-1.0E-10) 6,6,5
```

```
C***** CHECK IF MOLECULAR SPECIE POSSIBLE
```

```
6 IF(IPOS(I)) 44,5,44
```

```
C***** IF SPECIE IS POSSIBLE AND IS ZERO, EQUATE TO SMALL  
C***** POSITIVE QUANTITY.
```

```
44 YCOMP(I)=1.0E-6
```

```
IFLAG=1
```

```
5 CONTINUE
```

```
IF(IDBUG(12)-4) 807,804,804
```

```
804 IF(IFLAG) 805,805,806
```

```
805 WRITE(IWRIT,5003)
```

```
GO TO 807
```

```
806 WRITE(IWRIT,5004)(YCOMP(I),I=1,NGMS)
```

```
807 CONTINUE
```

```
RETURN
```

```
C***** IF A POSITIVE SET HAS NOT BEEN GENERATED (KINIT=0)  
C***** , SET IPOS ELEMENTS ZERO FOR ANY ZERO SPECIES.
```

```
900 DO 901 I=1,NGMS
```

```
IF(YCCMP(I)-1.0E-10) 902,902,901
```

```
902 IPOS(I)=0
```

```
901 CONTINUE
```

```
RETURN
```

```
5000 FORMAT(1H0,'INITIAL MOLE NUMBERS ARE -'/(6E15.7))
```

```
5001 FORMAT(1H0,'IPOS VECTOR IS ',20I4)
```

```
5002 FORMAT(1H0,'B'S ARE ',5E15.7)
```

```
5003 FORMAT(1H0,'POSITIVE SET EXISTS' )
```

```
5004 FORMAT(1H0,'POSITIVE SET GENERATED IS -'/(6E15.7))
```

```
5005 FORMAT(1H0,' FREE ENERGY FUNCTIONS (F/RT + LN P) ARE  
$-'/(5E15.7))
```

```
END
```



```

C *****
C *
C *          SUBROUTINE YMODY
C *
C * FUNCTIONS -
C *
C * - COMPOSITION MODIFICATION ROUTINE
C * - PREVENTS NEGATIVE OR PREMATURELY ZERO MOLE
C *   NUMBERS DURING ENERGY MINIMIZATION
C * - DEFINES NEW MOLE NUMBERS AND CHECKS FOR
C *   CONVERGENCE OF THE COMPOSITION CALCULATIONS
C * - EQUATES SPECIES DRIVEN BELOW A SPECIFIED LEVEL
C *   (I.E. 1.E-10) TO ZERO AND FLAGS THEM SO THEY WILL
C *   BE IGNORED (THIS SPEEDS CONVERGENCE)
C *
C *****

```

```

SUBROUTINE YMODY(YCOMP,ADD,ICNT,ITER,TDEGF,PRESS,IPOS)
DOUBLE PRECISION FAC,FAC1,YCOMP,ADD
DIMENSION ADD(20),YCOMP(20),IPOS(20)
COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /DATA2/NAME(20,4)

```

```

C*****      HERE TO 8 -
C*****      CHECK TO SEE IF ANY MOLE NUMBERS WILL BECOME
C*****      NEGATIVE WHEN THE CALCULATED CORRECTIONS ARE
C*****      MADE. IF NOT USE EXISTING CHANGES. IF SOME WILL
C*****      BECOME NEGATIVE OR ZERO, FIND FAC1 (WHICH THE
C*****      CORRECTIONS ARE MULTIPLIED BY) SUCH THAT NONE OF
C*****      THE MOLE NUMBERS BECOME ZERO OR NEGATIVE.

```

```

FAC1=1.0
DO 8 I=1,NGMS

```

```

C*****      IF IPOS=0 , IGNORE THAT MOLECULAR SPECIE
C*****      (IE. EITHER PHYSICALLY IMPOSSIBLE OR ELSE HAS BEEN
C*****      DRIVEN TO ZERO)

```

```

      IF(IPOS(I)) 8,8,13
13 IF(YCOMP(I)+ADD(I)) 9,9,8
  9 FAC=0.99*DABS(YCOMP(I)/ADD(I))
    IF(FAC-FAC1) 12,8,8
12 FAC1=FAC
  8 CONTINUE

```

```

C*****      HERE TO 10 - FIND NEW MOLE NUMBERS AND CHECK FOR
C*****      CONVERGENCE

```

```

ICNT=0
DO 10 I=1,NGMS

```

```

C*****      IF IPOS=0 , IGNORE THAT MOLECULAR SPECIE

```


SUBROUTINE YMODY ... (CONT'D)

```
IF(IPOS(I)) 11,11,14
```

```
C*****  MODIFY CORRECTIONS (IF NECESSARY) SUCH THAT MOLE
C*****  NUMBERS WILL NOT BECOME ZERO OR NEGATIVE.
```

```
14 ADD(I)=ADD(I)*FAC1
```

```
C*****  FIND NEW MOLE NUMBERS
```

```
YCOMP(I)=YCOMP(I)+ADD(I)
```

```
C*****  IF MOLE NUMBER HAS BEEN DRIVEN BELOW A SPECIFIED
C*****  VALUE, EQUATE MOLE NUMBER TO ZERO AND SET IPOS=0
C*****  FOR THAT SPECIE SO THAT IT WILL BE IGNORED FOR THE
C*****  REMAINDER OF THE MINIMIZATION. THIS CAN SPEED UP
C*****  CONVERGENCE CONSIDERABLY.
```

```
IF(YCOMP(I)-1.0E-10) 20,20,21
20 IPOS(I)=0
YCOMP(I)=0.0
GO TO 11
```

```
C*****  IF RELATIVE CHANGE IN THE MOLE NUMBER IS LESS THAN
C*****  A SPECIFIED VALUE, INCREMENT CONVERGENCE COUNTER
C*****  (ICNT). THIS COUNTER IS ALSO INCREMENTED FOR
C*****  'IGNORED' SPECIES, SO THAT WHEN THE COMPOSITION
C*****  HAS CONVERGED, ICNT=NGMS, OTHERWISE IT IS LESS
C*****  THAN NGMS.
```

```
21 IF(DABS(ADD(I)/YCOMP(I))-CRIT) 11,11,10
11 ICNT=ICNT+1
10 CONTINUE
IF(IDBUG(12)-7) 805,804,804
804 WRITE(IWRIT,5002) ITER,FAC1,ICNT,(YCOMP(I),I=1,NGMS)
805 CONTINUE
IF(ICNT-NGMS) 101,100,100
100 CONTINUE
IF(IDBUG(12)-1) 801,800,800
800 WRITE(IWRIT,5000) TDEGF,PRESS,CRIT,ITER
801 IF(IDBUG(12)-3) 803,802,802
802 WRITE(IWRIT,5001) ((NAME(I,J),J=1,4),YCOMP(I),I=1
$,NGMS)
803 CONTINUE
101 RETURN
5000 FORMAT(1H ' CONVERGENCE OBTAINED AT ',F9.2,' DEG. F,
$, PRESSURE= ',
1 F6.2,' PSIA'/10X,' CRIT = ',E9.2,' ITERATIONS = '
$,I4/)
5001 FORMAT(1H ', ' THE CONVERGED MOLE NUMBERS ARE AS FOLLOWS
$ - '//(' ',
```


SUBROUTINE YMODY ... (CONT'D)

```
14A1,' - ',F15.7,5X,4A1,' - ',F15.7,5X,4A1,' - '  
$,F15.7))  
5002 FORMAT(1H0,'ITER = ',I4,', FAC1 = ',E15.7,',  
$ ICNT = ',I3,  
1', Y'S ARE -' /(6E15.7))  
END
```



```

C *****
C *
C *          SUBROUTINE GAUSS
C *
C * FUNCTIONS -
C *
C * - GAUSSIAN ELIMINATION ROUTINE
C * - SOLVES THE GIVEN MATRIX EQUATION FOR THE
C *   LAGRANGIAN MULTIPLIERS
C * - PARTIAL PIVOTTING IS USED TO REDUCE ROUND-OFF
C *   ERRORS DURING CALCULATIONS
C * - SINGULARITY OF THE MATRIX RESULTS IN JOB
C *   TERMINATION
C *
C *****

```

```

      SUBROUTINE GAUSS (A,R,N,X)
      DOUBLE PRECISION A,R,X,U,S
      DIMENSION A(6,6),R(6),X(6)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT

```

```

C*****      SOLUTION OF N SIMULTANEOUS LINEAR EQUATIONS USING
C*****      GAUSSIAN ELIMINATION - PARTIAL PIVOTING IS USED
C*****      TO REDUCE ROUND-OFF ERROR (MATRIX FORM AX=R)

```

```

      M=N-1

```

```

C*****      HERE TO 11 TRIANGULARIZE THE MATRIX

```

```

      DO 11 J=1,M
      S=0.0

```

```

C*****      HERE TO 12 - FIND THE PIVOTAL ELEMENT

```

```

      DO 12 I=J,N
      U=DABS(A(I,J))
      IF(U-S) 12,12,112
112 S=U
      L=I
12 CONTINUE

```

```

C*****      HERE TO 19 - EXCHANGE ROWS IF NECESSARY

```

```

      IF(L-J) 119,19,119
119 DO 14 I=J,N
      S=A(L,I)
      A(L,I)=A(J,I)
14 A(J,I)=S
      S=R(L)
      R(L)=R(J)
      R(J)=S

```


SUBROUTINE GAUSS ... (CONT'D)

C***** CHECK FOR SINGULARITY

```
19 IF(DABS(A(J,J))-1.0E-30) 115,115,15
115 WRITE(IWRIT,3)
    CALL EXIT
```

C***** HERE TO 11 COMPLETE THE PIVOTAL OPERATION

```
15 MM=J+1
    DO 11 I=MM,N
        IF(DABS(A(I,J))-1.0E-30) 11,111,111
111 S=A(J,J)/A(I,J)
    A(I,J)=0.0
    DO 16 K=MM,N
16  A(I,K)=A(J,K)-S*A(I,K)
    R(I)=R(J)-S*R(I)
11 CONTINUE
```

C***** HERE TO 17 - HAVING TRIANGULARIZED THE MATRIX,
C***** FIND SOLUTION VECTOR , X, BY BACK SUBSTITUTION
C***** STARTING FROM BOTTOM.

```
    DO 17 K=1,N
        I=N+1-K
        S=0.0
        IF(I-N) 117,17,117
117 MM=I+1
        DO 18 J=MM,N
18  S=S+A(I,J)*X(J)
17  X(I)=(R(I)-S)/A(I,I)
    RETURN
3  FORMAT(1H , 'MATRIX SINGULAR')
    END
```



```

C *****
C *
C *          SUBROUTINE FAKER
C *
C *  FUNCTIONS -
C *
C *  - EQUILIBRIUM COMPOSITION MASK ROUTINE
C *  - IF 'NDUMY' IS NON-ZERO, TEMPORARILY SETS THE
C *    NUMBER OF GASEOUS MOLECULAR SPECIES TO NDUMY.
C *    (I.E. THE FIRST NDUMY SPECIES ARE NOT MASKED,
C *    AND THE LAST (NGMS-NDUMY) SPECIES ARE MASKED, OR
C *    IGNORED DURING THE COMPOSITION CALCULATION WHICH
C *    IMMEDIATELY FOLLOWS)
C *  - MASKING OCCURS ONLY IF BOILER OR CONVERTER
C *    COMPOSITIONS ARE BEING CALCULATED, AND ONLY IF
C *    THE TEMPERATURE (AT WHICH THE COMPOSITION IS TO
C *    BE CALCULATED) IS LOWER THAN THE SPECIFIED
C *    SECONDARY CUTOFF TEMPERATURE (TDUMY).
C *
C *****

```

```

SUBROUTINE FAKER(NGMS,TCTOF,TEMP)
COMMON /EXTRA/NDUMY,TDUMY
DATA JFLAG/0/

```

```

C*****      IF NDUMY ZERO, RETURN.

```

```

      IF(NDUMY) 20,20,21
20 RETURN
21 CONTINUE

```

```

C*****      IF TCTOF ZERO OR NEGATIVE, SHIFT ON GIVEN STREAM
C*****      -- RETURN --

```

```

      IF(TCTOF) 3,3,4
3 RETURN

```

```

C*****      IF TCTOF +VE BUT LESS THAN 10, COMPLETE
C*****      EQUILIBRIUM CALCULATION , CHECK TEMP.

```

```

4 IF(TCTOF-10.) 5,5,7

```

```

C*****      IF TEMP G.T. 900. COMPLETE EQUIL. MAY BE CALC'D.
C*****      IF TEMP. L.T. 900, ASSUME CONVERTER (MASK
C*****      SPECIES)

```

```

5 IF(TEMP-900.) 6,6,3

```

```

C*****      MASK LAST GASEOUS SPECIES SO THEY ARE FROZEN

```

```

6 NGMS=NDUMY
  RETURN

```


SUBROUTINE FAKER ... (CONT'D)

C***** CHECK IF TEMP. IS G.T. SECONDARY CUTOFF TEMP.

7 IF(TEMP-TDUMY) 9,8,8

C***** FLAG TEMP. GREATER THAN SEC. CUTOFF.

8 JFLAG=1
RETURN

C***** CHECK HIGH TEMP. FLAG

9 IF(JFLAG) 6,6,10

C***** SET PRIMARY CUTOFF TO SECONDARY CUTOFF FOR
C***** A SINGLE COMPOSITION CALCULATION - LAST
C***** COMPONENTS WILL BE MASKED FOR NEXT COMP. CALC.

10 TCTOF=TDUMY

C***** RESET HIGH TEMP. FLAG

JFLAG=0
RETURN
END


```

C *****
C *
C *          SUBROUTINE INPUT
C *
C * FUNCTIONS -
C *
C * - DATA INPUT EXECUTIVE ROUTINE
C * - INITIALIZES DATA INPUT AND THEN READS ALL
C *   DATA USING 'FFINP' FREE FORMAT INPUT ROUTINE
C * - FOR EACH DATA SEGMENT OF INPUT, TRANSFERS
C *   CONTROL TO APPROPRIATE INPUT SUBROUTINE--
C *   THIS ROUTINE IS DETERMINED FROM DECODED DATA
C *   CONTROL MESSAGES
C * - IF ANY ERRORS ARE DETECTED DURING DATA INPUT,
C *   THE JOB IS ABORTED WHEN DATA INPUT IS COMPLETE
C *
C *****

```

```

SUBROUTINE INPUT
  DIMENSION TREF(10)
  COMMON /GEN1/IWRIT, IDBUG(15), ITFST, CRIT, NGMS, NTOT
  COMMON /EXEC1/JTYPE(25), INDEX(25), ISEQ(25), IASUM(25)
  $, ISUPR, IOPT
  COMMON /FLOW1/INFO(75,5), NNEQP, NOSTM
  COMMON /INPUT1/IV(25), RV(25), IALPH(50), NI, NR, NA, NOXEQ
  COMMON /INPUT2/ISYMB(20), IATOM(5), ATMWT(5), VATOM(5)
  $, KEQIV(20)
  DATA TREF/-840192., -912384., -757760., -569856., -415232.
  $, -672768.,
  1 -371456., 0., -90624., -357888./

```

```

C***** INITIALIZE FLAGS AND PARAMETERS

```

```

  IREAD=1
  IWRIT=8
  WRITE(IWRIT,9999)
9999 FORMAT('1'/////////T37'SULPHUR PLANT DESIGN AND
  $ SIMULATION'////////)
  NOXEQ=0
  IOPT=1
  ISUPR=0
  NGMS=0
  NTOT=0
  NOSTM=0
  KEQIV(1)=1
  ICHCK=0
  JCHCK=0

```

```

C***** INITIALIZE IDBUG VECTOR & CRIT IN CASE THEY'RE NOT
C***** READ FIRST.

```

```

DO 10 I=1,15

```


SUBROUTINE INPUT ... (CONT'D)

```

10 IDBUG(I)=0
   CRIT=1.0E-4
100 CONTINUE

```

```

C***** IF ECHO CHECK WANTED, SKIP TO NEW PAGE.

```

```

      IF(IDBUG(14)-1) 801,800,800
800 WRITE(IWRIT,1003)
801 CONTINUE

```

```

C***** READ INPUT VIA FFIMP - (UNSPECIFIED INPUT).

```

```

110 KFLAG=0
   CALL FFIMP(IV,RV,IALPH,NI,NR,NA,IWRIT,IREAD,KFLAG
$,TVALU)

```

```

C***** SET INPUT FLAGS.

```

```

      IEND=0
      IND=0

```

```

C***** CHECK FOR FFIMP ERROR.

```

```

      IF(KFLAG) 500,101,101
500 WRITE(IWRIT,5000)
      NOXEQ=1
      KFLAG=0

```

```

C***** IDENTIFY CONTROL MESSAGE RETURNED (TVALU).

```

```

101 DO 102 I=1,10
      IF(ABS(TVALU-TREF(I))-ABS(TVALU/1000.)) 103,103,102
102 CONTINUE

```

```

C***** IF NOT IDENTIFIED, ERROR MESSAGE, THEN TRY AGAIN.

```

```

      WRITE(IWRIT,5001) TVALU
      NOXEQ=1
      GO TO 110

```

```

C***** GO TO APPROPRIATE INPUT ROUTINE.

```

```

103 GO TO (1,2,3,4,5,6,7,8,8,200),I

```

```

C***** INPUT OF PROGRAM CONTROL PARAMETERS.

```

```

      6 CALL INPT0
      GO TO 150

```

```

C***** INPUT OF MOLECULAR AND THERMODYNAMIC DATA.

```


SUBROUTINE INPUT ... (CONT'D)

```
1 CALL INPT1(IND,IEND)
  IF(IEND) 11,150,11
```

```
C***** DATA CALCULATIONS AND M & T DATA ECHO CHECK IF
C***** DESIRED.
```

```
11 CALL INPT2
   GO TO 150
```

```
C***** INPUT OF EQUIP. PARAMETER SPECS. (& DATA ECHO
C***** CHECK).
```

```
2 ISPEC=-1
  CALL INPT3(IND,ISPEC,ICHCK)
  GO TO 150
```

```
C***** INPUT OF EQUIP. PARAMETER ESTIMATES (& DATA ECHO
C***** CHECK).
```

```
3 ISPEC=1
  CALL INPT3(IND,ISPEC,ICHCK)
  GO TO 150
```

```
C***** INPUT OF STREAM SPECS. (& DATA ECHO CHECK).
```

```
4 ISPEC=-1
  CALL INPT4(IND,ISPEC,JCHCK,ICNT)
  GO TO 150
```

```
C***** INPUT OF STREAM ESTIMATES (& DATA ECHO CHECK).
```

```
5 ISPEC=1
  CALL INPT4(IND,ISPEC,JCHCK,ICNT)
  GO TO 150
```

```
C***** INPUT OF FLOWSHEET DATA (& DATA ECHO CHECK).
```

```
7 CALL INPT5(IND)
  GO TO 150
8 WRITE(IWRIT,5004)
  GO TO 110
```

```
C***** IF END OF DATA SET, LOOK FOR NEW DATA SET CONTROL
C***** CARD. IF END OF ALL DATA, TERMINATE. IF NEITHER,
C***** CONTINUE WITH INPUT.
```

```
150 IF(IEND) 200,151,201
```

```
C***** READ MORE INPUT VIA FFIMP. (UNSPECIFIED INPUT).
```


SUBROUTINE INPUT ...(CONT'D)

```

151 KFLAG=0
    CALL FFINP(IV,RV,IALPH,NI,NR,NA,IWRIT,IREAD,KFLAG
$,TVALU)

C*****      CHECK FOR FFINP ERROR.

    IF(KFLAG) 502,152,152
502 WRITE(IWRIT,5002) I
    NOXEQ=1
    KFLAG=0

C*****      CHECK FOR END OR END OF ALL DATA CONTROL MESSAGE.-
C*****      ANY OTHER CONTROL MESSAGE RESULTS IN INPUT ERROR.
C*****      IF NO MESSAGE, GO TO ASSIGNMENT .

152 IF(TVALU) 153,103,153
153 IF(ABS(TVALU-TREF(9))-ABS(TVALU/1000.)) 159,159,154
154 IF(ABS(TVALU-TREF(10))-ABS(TVALU/1000.)) 158,158,503
503 WRITE(IWRIT,5003) TVALU
    NOXEQ=1
    KFLAG=0
    GO TO 101

C*****      SET FLAG FOR END OF DATA SET - GO TO ASSIGNMENT.

159 IEND= 1
    GO TO 103
201 WRITE(IWRIT,1001)
    GO TO 100

C*****      SET FLAG FOR END OF ALL DATA - GO TO ASSIGNMENT.

158 IEND=-1
    GO TO 103
200 WRITE(IWRIT,1000)
    CALL SPECL

C*****      IF ERROR IN DATA INPUT ENCOUNTERED (NOXEQ=1), CALL
C*****      EXIT. * OTHERWISE (NOXEQ=0) PROCEED TO
C*****      CALCULATION EXECUTIVE PROGRAM.

    IF(NOXEQ) 300,300,301
300 CONTINUE
    WRITE(6,1111)
    RETURN
301 WRITE(6,2222)
    CALL EXIT
1000 FORMAT('0',T25,'END OF ALL DATA')
1001 FORMAT('0',T25,'END')
1003 FORMAT('1'///)

```


SUBROUTINE INPUT ...(CONT'D)

```
1111 FORMAT('0'T25'NO ERRORS DETECTED IN INPUT DATA, ALL
$ SYSTEMS ARE GO
1 ' )
2222 FORMAT('0'T25'ERROR DETECTED IN INPUT DATA, NO GO ' )
5000 FORMAT(' ERROR ON FFIMP RETURN - INPUT CONTROL
$ CARD')
5001 FORMAT(' INVALID CONTROL CARD ENCOUNTERED - INPUT
$ CONTROL CARD,
1 TVALU = ',F15.7)
5002 FORMAT(' ERROR ON FFIMP RETURN - I = ',I3)
5003 FORMAT(' INVALID CONTROL CARD ENCOUNTERED - DATA
$ INPUT
1 TVALU = ',F15.7)
5004 FORMAT(' DATA CONTROL CARD MISSING OR *END* OUT OF
$ PLACE')
END
```



```

C *****
C *
C *          SUBROUTINE INPTO
C *
C *  FUNCTIONS -
C *
C *  - PROGRAM CONTROL PARAMETER DATA INPUT ROUTINE
C *  - SETS OUTPUT PRIORITY VECTOR (IDBUG) AND
C *  CONVERGENCE CRITERIA (CRIT) TO GIVEN OR
C *  DEFAULT VALUES
C *  - SETS 'PRINT SUPPRESS' AND 'NO OPTIMIZATION'
C *  FLAGS IF DESIRED
C *  - ECHO CHECKS THIS DATA IF DESIRED
C *    (IDBUG(14)=4 OR GREATER)
C *
C *****

```

```

SUBROUTINE INPTO
  DIMENSION TREF(3)
  DIMENSION R1(6),R2(6),R3(6),R4(6),R5(6),R6(6),R7(6)
  $,R8(6),
  1 R9(6),R10(6),R11(6),R12(6),R13(6),R14(6),R15(6),S(6
  $,15)
  COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
  COMMON /EXEC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
  $,ISUPR,IOPT
  COMMON /INPUT1/IV(25),RV(25),IALPH(50),NI,NR,NA,NOXFO
  EQUIVALENCE (R1(1),S(1)),(R2(1),S(7)),(R3(1),S(13))
  $,(R4(1),S(19)),
  1 (R5(1),S(25)),(R6(1),S(31)),(R7(1),S(37)),(R8(1)
  $,S(43)),
  1 (R9(1),S(49)),(R10(1),S(55)),(R11(1),S(61)),(R12(1)
  $,S(67)),
  1 (R13(1),S(73)),(R14(1),S(79)),(R15(1),S(85))
  DATA R1 /'WAST','E HE','AT R','DILE','R ',' ' '/'
  DATA R2 /'IN-L','INE ','BURN','ER ',' ' '/'
  DATA R3 /'CONV','ERTE','R ',' ' ',' ' '/'
  DATA R4 /'COND','FNSF','R ',' ' ',' ' '/'
  DATA R5 /'ADIA','BATI','C CO','MBIN','ER ',' ' '/'
  DATA R6 /'COMB','INER','/DIV','IDER',' ',' ' '/'
  DATA R7 /'COMB','USTI','ON A','IR A','DDER',' ',' ' '/'
  DATA R8 /'INCI','NERA','TOR ',' ',' ' '/'
  DATA R9 /'STAC','K ',' ',' ' ',' ' '/'
  DATA R10/'BLAC','K BO','X ',' ',' ' ',' ' '/'
  DATA R11/' ',' ',' ',' ',' ',' ' ',' ' '/'
  DATA R12/'EQUI','LIBR','IUM ','COMP','OSIT','ION '/'
  DATA R13/'CALC','ULAT','ION ','OPTI','MIZA','TION '/'
  DATA R14/'DATA',' INP','UT E','CHO ','CHEC','K '/'
  DATA R15/'EXEC','UTIV','E FU','NCTI','ONS ',' ' '/'
  DATA TREF,IBLNK/-342272.,-384512.,-726784., ' ' '/'

```

C***** CHECK FOR EXISTENCE OF INTEGER,REAL OR ALPHA DATA.

SUBROUTINE INPTO ... (CONT'D)

```

      IF(NI+NR+NA) 90,90,91
    90 RETURN
    91 IF(IV(14)-4) 803,802,802
    802 WRITE(IWRIT,1000)
    803 CONTINUE

```

C***** CHECK FOR EXISTENCE OF REAL DATA.

```

      IF(NR-1) 102,93,93

```

C***** CHECK THAT CRIT (REAL VALUE) IS BETWEEN 0 AND 1.

```

    93 IF(RV(1)-1.0) 100,100,501
   100 IF(RV(1)) 501,501,101
   501 WRITE(IWRIT,5001)
      NOXEQ=1
      GO TO 102
   101 CRIT=RV(1)

```

C***** CHECK FOR EXISTENCE OF INTEGER DATA.

```

    102 IF(NI) 103,103,104

```

C***** DEFINE ALL ELEMENTS OF IDBUG VECTOR.

```

    104 DO 105 I=1,NI

```

C***** CHECK THAT ELEMENT OF IDBUG IS IN RANGE 0-10.

```

      IF(IV(I)) 500,106,106
   106 IF(IV(I)-15) 105,105,500
   500 WRITE(IWRIT,5000)
      NOXEQ=1
   105 IDBUG(I)=IV(I)
   103 IF(NA) 110,110,107
   107 IF(IDBUG(14)-4) 805,804,804
   804 WRITE(IWRIT,1002) (IALPH(I),I=1,NA)
   805 CONTINUE
      TVALU=0.0
      IFACT=IBLNK/16448
      DO 120 I=1,NA
   120 TVALU=TVALU+(IALPH(I)-IBLNK)/IFACT
      DO 121 I=1,3
      IF(ABS(TREF(I)-TVALU)-ABS(TVALU/1000.)) 122,122,121
   121 CONTINUE
      WRITE(IWRIT,5002)
      NOXEQ=1
      GO TO 110
   122 GO TO (123,124,125),I
   123 ISUPR=1

```


SUBROUTINE INPTO ... (CONT'D)

```

      GO TO 126
124  IOPT=0
      GO TO 126
125  ISUPR=1
      IOPT=0
126  CONTINUE

```

C***** ECHO CHECK IF DESIRED.

```

110  IF(IDBUG(14)-4) 801,800,800
800  WRITE(IWRIT,1001) CRIT
      DO 200 I=1,15
200  WRITE(IWRIT,2000) I,IDBUG(I),(S(J,I),J=1,6)
801  CONTINUE
      RETURN
1000  FORMAT(///T35,'ECHO CHECK OF PROGRAM CONTROL
$ PARAMETERS'//)
1001  FORMAT(//T30'VAL',
1'UE OF THE CALCULATIONAL CRITERION IS ',F9.2/T26
$, '(ALL INTERNAL C
1ONVERGENCE CRITERIA ETC. ARE SCALED TO THIS)'////T29
$ 'IDBUG
1VALUE APPLICATION'//)
1002  FORMAT('0'/T25,80A1)
2000  FORMAT(T31,I2,5X,I3,7X,6A4)
5000  FORMAT('0 IDBUG ELEMENTS MUST BE IN RANGE 0-10')
5001  FORMAT('0 CRITERION (CRIT) MUST BE IN RANGE 0-1')
5002  FORMAT('0 INVALID ALPHAMERIC MESSAGE')
      END

```



```

C *****
C *
C *
C *          SUBROUTINE INPT1
C *
C *  FUNCTIONS -
C *
C *  -  MOLECULAR AND THERMODYNAMIC DATA INPUT ROUTINE
C *  -  INITIALIZES M AND T DATA -- SETS THE NUMBER
C *      OF ATOMS TYPES, AND THE ATOM SYMBOLS, WEIGHTS
C *      AND VOLUMES
C *  -  STORES THERMODYNAMIC DATA (NASA) CONSTANTS AND
C *      VISCOSITY COEFFICIENTS IF GIVEN -- IF VISCOSITY
C *      COEFFICIENTS ARE NOT GIVEN, SETS THEM TO DEFAULT
C *      VALUES
C *  -  DEFINES THE NUMBER OF GASEOUS MOLECULAR
C *      SPECIES (NGMS) AND THE TOTAL NUMBER OF SPECIES
C *      (NTOT)
C *  -  CHECKS VALIDITY OF MOLECULAR SPECIES FORMULAS
C *      AND GENERATES THE FORMULA MATRIX (FORMU)
C *
C *****

```

```

      SUBROUTINE INPT1(IND,IEND)
      DIMENSION NUMB(9)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /INPUT1/IV(25),RV(25),IALPH(50),NI,NR,NA,NOXEQ
      COMMON /INPUT2/ISYMB(20),IATOM(5),ATMWT(5),VATOM(5)
      $,KEQIV(20)
      COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)/DATA2/NAME(20
      $,4)
      COMMON /DATA3/TDATA(20,14)/DATA4/RMU(20),SMU(20)
      $,RADCT(20)
      DATA NUMB/'1 ','2 ','3 ','4 ','5 ','6 ','7 ','8 ','9 '
      $/
      DATA ILIQ,IBLNK,ISTAR/'L ',' ','* '/
      DATA VIS1,VIS2/0.015,0.000020/

```

```

C*****      CHECK FOR EXISTENCE OF REAL DATA.  IF SOME DOES,
C*****      CHECK IND.

```

```

      IF(NR) 91,90,91

```

```

C*****      IF END OF DATA SET, (IEND=1), DO DATA
C*****      CALCULATIONS. IF NOT, RETURN.

```

```

      90 IF(IEND) 205,200,205
      200 RETURN

```

```

C*****      IF FIRST MOLECULAR DATA (ATOM SYMBOLS, WEIGHTS AND
C*****      VOLUMES) THEN INITIALIZE DATA INPUT.

```

```

      91 IF(IND) 92,92,95

```


SUBROUTINE INPT1 ... (CONT'D)

92 IND=1

C***** INITIALIZE NUMBER OF GASEOUS MOLECULAR SPECIES
C***** (NGMS) AND NUMBER OF LIQUID MOLECULAR SPECIES
C***** (NLMS) TO ZERO.

NGMS=0

NLMS=0

C***** CHECK FOR MORE THAN 5 ATOMIC SPECIES.

IF(NA-5) 102,102,155

155 WRITE(IWRIT,5005)

NOXEQ=1

NR=5

C***** CHECK FOR EQUAL ATOM TYPES ,WEIGHTS AND VOLUMES.

102 IF(NR-NA*2) 151,103,151

151 WRITE(IWRIT,5001)

NOXEQ=1

C***** DEFINE NUMBER OF ATOM TYPES (NATYP), ATOM TYPES
C***** (IATOM) AND ATOMIC WEIGHTS (ATMWT). THIS
C***** COMPLETES DATA INITIALIZATION.

103 NATYP=NA

DO 104 I=1,5

IATOM(I)=IALPH(I)

K=I*2

ATMWT(I)=RV(K-1)

VATOM(I)=RV(K)

104 CONTINUE

CC***** RETURN FOR MORE DATA.

RETURN

95 KASUM=0

C***** CHECK NUMBER OF REAL CONSTANTS READ. IF 14, ONLY
C***** THERMO. DATA GIVEN (MUST ASSUME VISCOSITY DATA).
C***** IF 16, BOTH THERMO AND VISCOSITY DATA GIVEN. ANY
C***** OTHER NUMBER INVALID.

IF(NR-14) 111,112,111

111 IF(NR-16) 153,113,153

153 WRITE(IWRIT,5003) (IALPH(IJ),IJ=1,4)

NOXEQ=1

112 KASUM=1

SUBROUTINE INPT1 ... (CONT'D)

```

C***** CHECK IF LIQUID COMPONENT. IF SO TEMPORARILY
C***** STORE AT END OF DATA VECTORS. IF NOT, ASSUME
C***** GASEOUS COMPONENT. INCREMENT APPROPRIATE COUNTER
C***** (NGMS OR NLMS).

```

```

113 IF (IALPH(NA)-ILIQ) 114,115,114
114 NGMS=NGMS+1
    NPLAC=NGMS
    GO TO 116
115 NLMS=NLMS+1
    NPLAC=21-NLMS

```

```

C***** CHECK FOR TOO MANY COMPONENTS.

```

```

116 IF (NGMS+NLMS-20) 119,119,554
554 WRITE (IWRIT,5004)
    NOXEQ=1
    NLMS=0
    IF (NGMS-20) 231,231,232
232 NGMS=20
231 RETURN
119 IWHER=NGMS+NLMS
    KEQIV(NPLAC)=IWHER

```

```

C***** SET VISCOSITY DATA TO THAT GIVEN OR ELSE ASSUME.
C***** ISYMB = '*' FOR ASSUMED COMPONENTS, ' ' OTHERWISE

```

```

    IF (KASUM) 117,117,118
117 RMU(NPLAC)=RV(1)
    SMU(NPLAC)=RV(2)
    ISYMB(NPLAC)=IBLNK
    INDIC=2
    GO TO 120
118 RMU(NPLAC)=VIS1
    SMU(NPLAC)=VIS2
    ISYMB(NPLAC)=ISTAR

```

```

C***** STORE THERMO. DATA

```

```

    INDIC=0
120 DO 121 I=1,14
    KNUMB=INDIC+I
121 TDATA(NPLAC,I)=RV(KNUMB)

```

```

C***** STORE SPECIES NAME (MAX. OF 4 ALPHA-NUM. FORMULA).

```

```

    DO 122 I=1,4
122 NAME(NPLAC,I)=IALPH(I)

```

```

C***** CHECK FOR POSSIBLE END OF DATA SET. IF SO DO, DO

```


SUBROUTINE INPT1 ... (CONT'D)

C***** DATA CALCULATIONS. OTHERWISE, RETURN FOR MORE
C***** DATA.

IF (IFND) 205,200,205
205 CONTINUE
NTOT=NGMS+NLMS

C***** INITIALIZE FORMULATION MATRIX.

DO 206 I=1,NTOT
DO 206 J=1,5
206 FORMU(I,J)=0.0

C***** IF ANY LIQ. COMPONENTS EXIST, RESTORE THEIR DATA
C***** RIGHT AFTER THE GASEOUS COMPONENT DATA.

IF (NLMS) 220,220,230
230 DO 211 I=1,NLMS
IND1=NGMS+I
IND2=20-NLMS+I
DO 212 J=1,14
212 TDATA(IND1,J)=TDATA(IND2,J)
RMU(IND1)=RMU(IND2)
SMU(IND1)=SMU(IND2)
ISYMB(IND1)=ISYMB(IND2)
KEQIV(IND1)=KEQIV(IND2)
DO 213 J=1,4
213 NAME(IND1,J)=NAME(IND2,J)
211 CONTINUE

C***** DEFINE FORMULATION MATRIX, USING GIVEN FORMULAS
C***** (NAMES) AND ATOMIC WEIGHTS.

220 DO 221 I=1,NTOT
KSTOR=0
DO 222 J=1,4
IF (NAME(I,J)-IBLNK) 228,222,228
228 DO 223 K=1,NATYP
IF (NAME(I,J)-IATOM(K)) 223,224,223
224 FORMU(I,K)=1.0
KSTOR=K
GO TO 222
223 CONTINUE

C***** IF FIRST CHARACTER OF FORMULA IS NUMERIC, ERROR.

IF (KSTOR) 225,156,225
156 WRITE(IWRIT,5006) (NAME(I,JJ),JJ=1,4)
NOXEQ=1
GO TO 221

SUBROUTINE INPT1 ... (CONT'D)

```

225 DO 226 K=1,9
    IF(NAME(I,J)-NUMB(K)) 226,227,226
227 FORMU(I,KSTOR)=FORMU(I,KSTOR)*K
    GO TO 222
226 CONTINUE

```

```

C*****  FORMULA CHARACTER HAS NOT BEEN IDENTIFIED -
C*****  INVALID ATOMIC SPECIE (NOT GIVEN) OR INVALID
C*****  NUMBER IN FORMULA (1-9 VALID).

```

```

    WRITE(IWRIT,5006) (NAME( I,JJ),JJ=1,4)
    NOXEQ=1
    GO TO 221
222 CONTINUE
221 CONTINUE
    RETURN
5001 FORMAT('O  ERROR IN ATOM NAMES, WEIGHTS AND VOLUMES
$ DATA.')
```

```

5003 FORMAT(1H0,' INVALID MOLECULAR DATA - WRONG NUMBER OF
$ CONSTANTS -
1  (' ,4A1,')')
5004 FORMAT(1H0,' TOO MANY MOLECULAR SPECIES GIVEN (LIMIT
$ IS 20)')
5005 FORMAT(1H0,' TOO MANY ATOM TYPES GIVEN (LIMIT IS 5)')
5006 FORMAT(1H0,' INVALID MOLECULAR FORMULATION GIVEN.- ('
$,4A1,')')
    END

```



```

C *****
C *
C *          SUBROUTINE INPT2
C *
C *  FUNCTIONS -
C *
C *  - MOLECULAR AND THERMODYNAMIC DATA ANALYSIS ROUTINE
C *  - CALCULATES MOLECULAR WEIGHTS AND VOLUMES
C *  - DEFINES WHICH SPECIES ARE RADIATING COMPONENTS
C *    (FOR HEAT LOSS CALCULATIONS) -- ASSUMES SPECIES
C *    WITH THREE OR MORE CONSTITUENT ATOMS ARE POLAR
C *    AND RADIATING
C *  - IDENTIFIES AND STORES WATER VAPOR COMPONENT
C *    AND SULPHUR VAPOR AND LIQUID COMPONENTS
C *  - ECHO CHECKS M AND T DATA IF DESIRED
C *    (IDBUG(14) = 3 OR GREATER)
C *
C *****

```

```

      SUBROUTINE INPT2
      DIMENSION NUMB(9)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /INPUT1/IV(25),RV(25),IALPH(50),NI,NR,NA,NOXEQ
      COMMON /INPUT2/ISYMB(20),IATOM(5),ATMWT(5),VATOM(5)
      $,KEQIV(20)
      COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)/DATA2/NAME(20
      $,4)
      COMMON /DATA3/TCDATA(20,14)/DATA4/RMU(20),SMU(20)
      $,RADCT(20)
      COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)
      DATA IS,IGAS,ILIQ,IBLNK,NUMB/'S ','G ','L ',' ','1 '
      $,'2 ','3 ','4
      1 ','5 ','6 ','7 ','8 ','9 ' /

```

```

C*****      DEFINE WTMOL AND RADCT.

```

```

      DO 240 I=1,NTOT
      WTMOL(I)=0.0
      RADCT(I)=0.0
      NATOM=0

```

```

C*****      CALCULATE MOLECULAR WEIGHTS (WTMOL), USING ATOMIC
C*****      WEIGHTS AND FORMULATION MATRIX.

```

```

      DO 232 J=1,5
      IF(FORMU(I,J)-1.0E-2) 232,232,231
231  WTMOL(I)=WTMOL(I)+FORMU(I,J)*ATMWT(J)
      NUMBR=FORMU(I,J)+0.5
      NATOM=NATOM+NUMBR
232  CONTINUE

```

```

C*****      SET RADCT=1 FOR RADIATING COMPONENT, =0

```


SUBROUTINE INPT2 ...(CONT'D)

C***** OTHERWISE. CRITERION FOR RADCT=1 IS THAT MOLECULE
C***** HAVE 3 OR MORE CONSTITUENT ATOMS.

IF(NATOM-3) 240,238,238
238 PADCT(I)=1.0
240 CONTINUE

C***** FIND GASEOUS MOLECULAR VOLUMES (VMOLE),
C***** USING ATOMIC VOLUMES (VATOM).

DO 250 I=1,NGMS
VMOLE(I)=0.0
DO 250 J=1,NATYP
250 VMOLE(I)=VMOLE(I)+FORMU(I,J)*VATOM(J)

C***** IDENTIFY WATER AND SULPHUR STREAMS.

ICNTS=0

C***** ZERO SULPHUR IDENTIFICATION VECTOR

DO 399 I=1,5
399 IDSUL(I)=0
DO 400 I=1,NTOT

C***** SULPHUR STREAM MUST HAVE ONLY 'S' OR NUMBER IN
C***** FORMULA.

DO 401 J=1,4
IF(NAME(I,J)-IS) 402,401,402
402 IF(NAME(I,J)-IBLNK) 407,401,407
407 DO 404 K=1,9
IF(NAME(I,J)-NUMB(K)) 404,401,404
404 CONTINUE
GO TO 405
401 CONTINUE

C***** STORE IDENTIFIED SULPHUR COMPONENT NUMBER.

ICNTS=ICNTS+1

C***** CHECK FOR TOO MANY SULPHUR COMPONENTS (MAX OF 5).

IF(ICNTS-5) 415,415,420
420 WRITE(IWRIT,5009)
NOXEQ=1
GO TO 400
415 IDSUL(ICNTS)=I

C***** WATER STREAM (ONLY ONE ALLOWED), MUST HAVE MOL.

SUBROUTINE INPT2 ... (CONT'D)

C***** WT. OF 18.

405 IF (ABS(WTMOL(I)-18.0)-1.0E-1) 406,406,400
 406 IDH2O=I
 400 CONTINUE

C***** HERE TO END - ECHO CHECK IF DESIRED (IDBUG(14))
 C***** G.E. 1)

IF (IDBUG(14)-3) 801,800,800
 800 CONTINUE

IPHAS=IGAS
 WRITE(IWRIT,1000)
 WRITE(IWRIT,2000) (IATOM(I),I=1,NATYP)
 WRITE(IWRIT,2001) (ATMWT(I),I=1,NATYP)
 WRITE(IWRIT,2002) (VATOM(I),I=1,NATYP)
 WRITE(IWRIT,2003)
 DO 301 I=1,NTOT
 IF(I-1-NGMS) 301,302,301
 302 IPHAS=ILIQ
 301 WRITE(IWRIT,1001) I,(NAME(I,J),J=1,4),IPHAS,WTMOL(I)
 \$,VMOLE(I),
 1 RADCT(I),RMU(I),SMU(I),ISYMB(I)
 WRITE(IWRIT,1005)
 WRITE(IWRIT,1002) IDH2O,(IDSUL(I),I=1,ICNTS)
 IF (IDBUG(14)-4) 801,802,802
 802 DO 500 K=1,11,10
 KL=K
 KT=K+9
 IF(KT-NTOT) 502,502,501
 501 KT=NTOT
 IF(KT-KL) 500,502,502
 502 WRITE(IWRIT,1003)
 DO 315 I=KL,KT
 315 WRITE(IWRIT,1004) (NAME(I,J),J=1,4),(TDATA(I,J),J=1
 \$,14)
 500 CONTINUE
 801 CONTINUE
 RETURN

1000 FORMAT(1H0/T32'ECHO CHECK OF MOLECULAR AND
 \$ THERMODYNAMIC DATA'////)

1001 FORMAT(T27,I2,4X,4A1,2X,A1,2X,F5.1,3X,F5.1,4X,F3.1,3X
 \$,F6.4,
 1 2X,F9.7,1X,A1)

1002 FORMAT('0'/T25'WATER COMPONENT = ',I3,' SULPHUR
 \$ COMPONENTS = ',5
 1I3//)

1003 FORMAT('1'/////T38'THERMODYNAMIC DATA - NASA FORMAT'
 \$/T35'FIRST 7
 1CONSTANTS FOR 300 TO 1000 DEG. K.'/T35'LAST 7

SUBROUTINE INPT2 ... (CONT'D)

```

$ CONSTANTS FOR 1000 T
10 5000 DEG. K. '/')
1004 FORMAT(/T25,4X,4A1,7X,3E15.7,/(T25,4E15.7))
1005 FORMAT('0'T30'VISCOSITY DATA IN FORM - MU(CP)=RMU+SMU
$*T DEG. F. '/')
1T37,'* DENOTES ASSUMED VISCOSITY CONSTANTS'//)
2000 FORMAT(T25'ATOM -'/T31'NAME',5X,5(A1,9X))
2001 FORMAT(T29'WEIGHT',2X,5(F6.2,4X))
2002 FORMAT(T29'VOLUME',2X,5(F6.2,4X))
2003 FORMAT(/////
1T25 'SPECIE *          MOLECULAR          *          *
$ VISCOSITY *'
1/T25'NUMBER  FORMULA  WEIGHT  VOLUME  RADCT    RMU
$  SMU'
1/T25'-----
$-----' /
1/)
5009 FORMAT('0  TOO MANY SULPHUR SPECIES -  MAXIMUM IS 5
$ ')
END

```



```

C *****
C *
C *          SUBROUTINE INPT3
C *
C *  FUNCTIONS -
C *
C *  -  EQUIPMENT PARAMETER SPECIFICATION AND ESTIMATION
C *      DATA INPUT ROUTINE
C *  -  INITIALIZES EQUIPMENT PARAMETER VECTOR 'EQUIP'
C *      ELEMENTS TO ZERO
C *  -  DEFINES EQUIPMENT NUMBERS AND CORRESPONDING
C *      TYPES -- ALLOCATES EQUIP VECTOR STORAGE
C *      REQUIRED FOR EACH NUMBER AND STORES LOCATION
C *      IN AN INDEX
C *  -  STORES EQUIPMENT NUMBERS IN CALCULATION
C *      SEQUENCE VECTOR AS ENCOUNTERED. (THIS VECTOR
C *      IS NORMALLY RE-ORDERED LATER DURING CALCULATION
C *      SEQUENCE OPTIMIZATION)
C *  -  STORES EQUIPMENT PARAMETER SPECIFICATIONS IN
C *      EQUIP AS NEGATIVE VALUES DURING SPECIFICATION
C *      PHASE-- EQUIP PARAMETER ESTIMATES AS POSITIVE
C *      VALUES DURING ESTIMATION PHASE
C *  -  ECHO CHECKS SPECIFICATIONS AND ESTIMATES IF
C *      DESIRED (IDBUG(14)=1 OR GREATER)
C *
C *****

```

```

      SUBROUTINE INPT3(IND,ISPEC,ICHCK)
      DIMENSION ITYPE(10)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /INPUT1/IV(25),RV(25),IALPH(50),NI,NR,NA,NOXEQ
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
      COMMON /EXFC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
      $,ISUPP,IOPT
      DATA ITYPE/28,5,8,12,3,2,6,7,8,1/

```

```

C*****      CHECK FOR EXISTENCE OF INTEGER DATA.  IF NONE,
C*****      RETURN.

```

```

      IF(NI) 91,91,90
      91 RETURN
      90 CONTINUE

```

```

C*****      CHECK IF INITIALIZATION HAS BEEN DONE (IND=1) OR
C*****      NOT (IND=0).

```

```

      IF(IND) 100,100,101

```

```

C*****      CHECK IF SPECIFICATION (ISPEC=-1) OR ESTIMATION
C*****      (ISPEC=1).

```


SUBROUTINE INPT3 ...(CONT'D)

```
100 IF(ISPEC) 102,102,103
```

```
C***** SPECIFICATION INITIALIZATION.
C***** HERE TO 103 - DEFINE EQUIP. VECTOR INDEX.
C***** FIRST DATA (EQUIP. SPECIFICATION) WILL BE PAIRED
C***** EQUIP. NUMBERS AND EQUIP. TYPES. SET INDEX FOR
C***** EQUIP'S AS ENCOUNTERED SUCH AS TO LEAVE ENOUGH
C***** ROOM FOR EACH PIECE OF EQUIP. (DEPENDENT UPON
C***** EQUIP. TYPE).
C***** FOR EQUIP. NO. 'I', THE STARTING POINT FOR THE
C***** STORAGE OF EQUIP. PARAMETERS (IN EQUIP.) IS GIVEN
C***** BY THE ITH ELEMENT OF INDEX.
```

```
102 KPLAC=0
DO 1 I=1,25
  JTYPE(I)=0
  ISEQ(I)=0
1 INDEX(I)=-1
DO 2 I=1,300
2 EQUIP(I)=0.0
```

```
C***** CHECK FOR TOO MANY PIECES OF EQUIP (MAX 25).
```

```
IF(NI-50) 5,5,504
504 WRITE(IWRIT,5004)
NOXFQ=1
NI=50
```

```
C***** CHECK FOR EQUAL NUMBER OF EQUIP. NO.S AND TYPES.
```

```
5 IF(NI/2-(NI+1)/2) 502,6,502
502 WRITE(IWRIT,5002)
NOXFQ=1
NI=NI-1
```

```
C***** DEFINE THE NUMBER OF PIFCES OF EQUIP , NNEQP.
```

```
6 NNEQP=NI/2
DO 10 I=2,NI,2
  ICNT=I/2
  IALPH(ICNT)=KPLAC
  IDUM1=IV(I-1)
```

```
C***** ISEQ(I) IS THE ITH PIECE OF EQUIP ENCOUNTERED.
C***** THIS SEQUENCE WILL BE USED AS THE INITIAL EQUIP.
C***** CALCULATION ORDERING (OPTIMIZED LATER.).
```

```
ISEQ(ICNT)=IDUM1
```

```
C***** CHECK FOR VALID EQUIP NO. (1-25).
```


SUBROUTINE INPT3 ... (CONT'D)

```

      IF (IDUM1-25) 11, 11, 505
505  WRITE(IWRIT, 5005)
      NOXFQ=1
      IDUM1=25
11  IDUM2=IV(I)

```

```

C*****      CHECK FOR VALID EQUIP. TYPE. (LESS THAN 10 AND
C*****      ITYPE NOT ZERO)

```

```

      IF (IDUM2-10) 20, 20, 506
20  IF (ITYPE(IDUM2)) 506, 506, 12
506  WRITE(IWRIT, 5006)
      NOXEQ=1
      IDUM2=10

```

```

C*****      JTYPE VECTOR STORES EQUIP TYPES.

```

```

12  JTYPE(IDUM1)=IDUM2
      INDEX(IDUM1)=KPLAC

```

```

C*****      DEFINE INDEX ELEMENT FOR NEXT EQUIP. TO BE STORED
C*****      IN EQUIP. PARAMETER VECTOR, DEPENDING UPON ROOM
C*****      NEEDED FOR PRESENT EQUIP.

```

```

      KPLAC=KPLAC+ITYPE(IDUM2)

```

```

C*****      CHECK FOR EQUIP. VECTOR OVERFLOW.

```

```

      IF (KPLAC-300) 10, 10, 503
503  WRITE(IWRIT, 5003)
      NOXEQ=1
      KPLAC=275
10  CONTINUE
      ICHCK=1
103  IND=1

```

```

C*****      CHECK IF ECHO CHECK DESIRED.

```

```

      IF (IDBUG(14)-1) 801, 800, 800
800  IF (ISPEC) 802, 802, 803

```

```

C*****      INITIALIZATION OF EQUIP. PAR. SPECIFICATION ECHO
C*****      CHECK .

```

```

802  WRITE(IWRIT, 1003)
      WRITE(IWRIT, 1000) (IV(I), I=1, NI, 2)
      WRITE(IWRIT, 1006) (IV(I), I=2, NI, 2)
      WRITE(IWRIT, 1002) (IALPH(I), I=1, NNEQP)
      WRITE(IWRIT, 1004)
      ILINE=((NNEQP+9)/10)*3+16

```


SUBROUTINE INPT3 ...(CONT'D)

```

801 CONTINUE
   IF(ISPEC) 104,104,101
104 RETURN

```

```

C*****   EQUIP. PAR. ESTIMATION ECHO CHECK INITIALIZATION.

```

```

803 WRITE(IWRIT,1005)
   WRITE(IWPIT,1004)
   ILINE=16

```

```

C*****   CHECK TOO SEE THAT INITIALIZATION WAS DONE
C*****   (SPECIFICATION).

```

```

   IF(ICHCK) 551,551,550
551 WRITE(IWRIT,5007)
   NOXEQ=1
   RETURN
550 CONTINUE

```

```

C*****   CHECK FOR EXISTENCE OF ESTIMATION DATA.  IF NONE
C*****   ,RETURN.

```

```

   IF(NR) 801,801,101

```

```

C*****   STORE GIVEN DATA IN EQUIP VECTOR.

```

```

101 NMBEQ=IV(1)

```

```

C*****   CHECK FOR VALID NUMBER OF PAR. NO.'S AND VALUES.

```

```

   IF(NI-NR-1) 501,120,501
501 WRITE(IWRIT,5001) NMBEQ
   NOXEQ=1
   RETURN

```

```

C*****   CHECK FOR VALID EQUIP NO.

```

```

120 IF(INDEX(NMBEQ)) 902,700,700
902 WRITE(IWRIT,2001) NMBEQ
   NOXEQ=1
   RETURN

```

```

C*****   DEFINE MAX. PAR. NO. FOR THAT TYPE OF EQUIP.

```

```

700 IIIII=JTYPE(NMBEQ)
   IMAX=ITYPE(IIIII)
   KPLAC=INDEX(NMBEQ)
   DO 201 I=1,NR

```

```

C*****   DEFINE PARAMETER NUMBER

```


SUBROUTINE INPT3 ... (CONT'D)

JDUM=IV(I+1)

C***** CHECK FOR VALID EQUIP. PAR. NO. (DEPENDS UPON
C***** EQUIP. TYPE).

IF(JDUM-IMAX)701,701,901
901 WRITE(IWRIT,2000) NMBEQ,JDUM
NOXEQ=1
GO TO 201

C***** CHECK IF GIVEN PARAMETER HAS BEEN PREVIOUSLY
C***** GIVEN. (EQUIP ENTRY NON-ZERO, ERROR).

701 NPLAC=KPLAC+JDUM
IF(ABS(EQUIP(NPLAC))-1.0E-10) 200,200,500
500 WRITE(IWRIT,5000) IV(1),IV(I+1)
NOXEQ=1

C***** STORE IN EQUIP. MATRIX. (SPECIFICATION -VE,
C***** ESTIMATE +VE)

200 PVALU=RV(I)*ISPEC
201 EQUIP(NPLAC)=PVALU

C***** ECHO CHECK IF DESIRED.

IF(IDBUG(14)-1) 805,804,804
804 ILINE=ILINE+1+NR
IF(ILINE-54) 815,815,814
814 WRITE(IWRIT,3333)
3333 FORMAT('1')
WRITE(IWRIT,1004)
ILINE=6+NR
815 CONTINUE
WRITE(IWRIT,1007) IV(1),(IV(I+1),RV(I),I=1,NR)
805 CONTINUE
RETURN
2000 FORMAT(1H,'INDEX ERROR '2I4)
2001 FORMAT('0 INVALID EQUIP. NO. -',I6)
5000 FORMAT(' EQUIP. NO. 'I3,' PARAMETER NO. ',I3,' GIVEN
\$ MULTIPLY')
5001 FORMAT('0 FOR EQUIP. NO. 'I3' EQUIP. PAR. NO. 'S'/
1'AND PARAMETER VALUES DON'T MATCH.')

5002 FORMAT('0 EQUIP NO. 'S AND EQUIP TYPES DON'T MATCH')

5003 FORMAT('0 EQUIP. PARAMETER VECTOR HAS BEEN
\$ OVERFLOWED.')

5004 FORMAT('0 TOO MANY PIECES OF EQUIP - MAX OF 25')

5005 FORMAT('0 INVALID EQUIP. NO. (MUST BE L.F. 25)')

5006 FORMAT('0 INVALID EQUIP. TYPE (NO SUBROUTINE
\$ RECORDED)')

SUBROUTINE INPT3 ... (CONT'D)

```

5007 FORMAT('O SPECIFICATION MUST BE DONE BEFORE
$ ESTIMATION')
1003 FORMAT('O'//T29 'ECHO CHECK OF EQUIPMENT PARAMETER
$ SPECIFICATION
1DATA'//)
1004 FORMAT(/////T30, 'EQUIPMENT PARAMETER
$ PARA
1METER'/T31 'NUMBER NUMBER
$ VALUE'/
1/)
1005 FORMAT('O'// T30, 'ECHO CHECK OF EQUIPMENT PARAMETER
$ ESTIMATION DAT
1A'//)
1000 FORMAT('O'T25, 'EQUIP. NO. - ', (T45,10I4))
1006 FORMAT(' 'T25, 'EQUIP. TYPE - ', (T45,10I4))
1002 FORMAT(' 'T25, 'EQUIP. INDEX - ', (T45,10I4))
1007 FORMAT('O', T31, I3, (T51, I3, 13X, E15.7))
END

```



```

C *****
C *
C *          SUBROUTINE INPT4
C *
C * FUNCTIONS -
C *
C * - STREAM SPECIFICATIONS AND ESTIMATES DATA INPUT
C * ROUTINE
C * - INITIALIZES STREAM MATRIX (STREM) ELEMENTS TO
C * ZERO
C * - STORES STREAM SPECIFICATIONS AS NEGATIVE VALUES
C * IN STREM, STREAM ESTIMATES (DURING ESTIMATES
C * INPUT) AS POSITIVE VALUES
C * - ECHO CHECKS SPECIFICATIONS AND ESTIMATES
C * (SEPARATE INPUT DATA SECTIONS) IF THIS IS DESIRED
C * (IDBUG(14)=2 OR GREATER)
C *
C *****

```

```

SUBROUTINE INPT4(IND,ISPEC,JCHCK,ICNT)
COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /INPUT1/IV(25),RV(25),IALPH(50),NI,NR,NA,NOXEQ
COMMON /STOR1/EQUIP(300),ILOC,NMBFQ,STREM(50,22)
$,NSIN(5),NSOUT(5)
DATA IBRC1,IBRC2/'( ',' ) '/

```

```

C***** CHECK FOR EXISTENCE OF REAL DATA. IF NONE,
C***** RETURN.

```

```

IF(NR) 90,90,91
90 RETURN

```

```

C***** CHECK IF INITIALIZATION HAS BEEN DONE (IND=1) OR
C***** NOT (IND=0).

```

```

91 IF(IND) 100,100,101

```

```

C***** SPECIFICATION (ISPEC=-1) OR ESTIMATION (ISPEC=1).

```

```

100 IF(ISPEC) 102,102,103

```

```

C***** STREAM PARAMETER SPECIFICATION INITIALIZATION -
C***** ZERO THE STREAM MATRIX (STREM).

```

```

102 ICNT=0
DO 1 I=1,50
DO 1 J=1,22
1 STREM(I,J)=0.0
JCHCK=1

```

```

103 IND=1

```

```

C***** CHECK TOO SEE THAT INITIALIZATION WAS DONE

```


SUBROUTINE INPT4 ... (CONT'D)

C***** (SPECIFICATION).

```

      IF(JCHCK) 551,551,550
551  WRITE(IWRIT,5007)
      NOXEQ=1
      RETURN
550  CONTINUE

```

C***** IF ECHO CHECK DESIRED, INITIALIZE IT.

```

      IF(IDBUG(14)-2) 801,800,800
800  IF(ISPEC) 105,105,104
105  WRITE(IWRIT,1000)
      WRITE(IWRIT,1002)
      GO TO 301
104  WRITE(IWRIT,1001)
      WRITE(IWRIT,1002)
801  ILINE=11

```

C***** INPUT OF STREAM PARAMETERS (SPECS. OR ESTIMATES.).

```

101  IDUM=IV(1)

```

C***** CHECK FOR VALID STREAM NUMBER. (FIRST INTEGER,
C***** MUST BE 1-50).

```

      IF(IDUM) 504,504,200
200  IF(IDUM-50) 201,201,504
504  WRITE(IWRIT,5004)
      NOXEQ=1
      RETURN

```

C***** CHECK IF WHOLE STREAM GIVEN (ONLY ONE INTEGER =
C***** STRM. NO.) OR ONLY PART OF THE STREAM (MORE THAN
C***** ONE INTEGER = STRM. NO. AND STREAM PARAMETER
C***** NUMBERS).

```

201  IF(NI-1) 62,50,62

```

C***** CHECK IF WHOLE STREAM GIVEN BEFORE. IF SO, CHECK
C***** FOR CONSISTENT NO. OF STREAM PARAMETERS. IF NOT,
C***** SET NO. OF STREAM PARAMETERS FOR FUTURE REF.
C***** (ICNT).

```

      50  IF(ICNT) 52,51,52
      51  ICNT=NR
      52  IF(ICNT-NR) 501,53,501

```

C***** INCONSISTENT DATA.

SUBROUTINE INPT4 ... (CONT'D)

```
501 WRITE(IWRIT,5001)
      NOXEQ=1
```

```
C***** CHECK FOR TOO MANY PARAMETERS.
```

```
53 IF(NR-22) 54,54,506
506 WRITE(IWRIT,5006)
      NOXEQ=1
      RETURN
```

```
C***** STORE COMPOSITION (ALL BUT LAST TWO PARAMETERS).
```

```
54 ICOMP=NR-2
DO 56 JDUM=1,ICOMP
```

```
C***** CHECK THAT DATA NOT GIVEN BEFORE.
```

```
IF(ABS(STREM(IDUM,JDUM))-1.0E-6) 55,55,502
502 WRITE(IWRIT,5000) IDUM,JDUM
      NOXEQ=1
```

```
C***** STORE DATA (-VE FOR SPECIFICATION, +VE FOR
C***** ESTIMATION)
```

```
55 STREM(IDUM,JDUM)=RV(JDUM)*ISPEC
```

```
C***** FILL IV VECTOR FOR POSSIBLE ECHO CHECK PRINT-OUT.
```

```
56 IV(JDUM+1)=JDUM
```

```
C***** STORE TEMP. IN COLUMN 21 - CHECK NOT GIVEN
C***** BEFORE.
```

```
IF(ABS(STREM(IDUM,21))-1.0E-6) 57,57,507
507 JDUM=21
      WRITE(IWRIT,5000) IDUM,JDUM
      NOXEQ=1
```

```
C***** STORE DATA (-VE FOR SPECIFICATION, +VE FOR
C***** ESTIMATION)
```

```
57 STREM(IDUM,21)=RV(NR-1)*ISPEC
      IV(NR)=21
```

```
C***** STORE PRESS. IN COLUMN 22 - CHECK NOT GIVEN
C***** BEFORE.
```

```
IF(ABS(STREM(IDUM,22))-1.0E-6) 58,58,508
508 JDUM=22
      WRITE(IWRIT,5000) IDUM,JDUM
```


SUBROUTINE INPT4 ...(CONT'D)

NOXEQ=1

C***** STORE DATA (-VE FOR SPECIFICATION, +VE FOR
C***** ESTIMATION)

58 STREM(IDUM,22)=RV(NR)*ISPEC
IV(NR+1)=22
GO TO 70

C***** ONLY PART OF STREAM GIVEN
C***** CHECK THAT PARAMETERS AND PARAMETER NO.'S MATCH.

62 IF(NI-1-NR) 503,60,503
503 WRITE(IWRIT,5003)
NOXEQ=1
RETURN

C***** STORE PARAMETERS IN LOCATIONS GIVEN (PAR. NO.'S.).

60 DO 61 I=2,NI
JDUM=IV(I)

C***** CHECK THAT PARAMETER NUMBER IS VALID (1-22).

IF(JDUM) 505,505,202
202 IF(JDUM-22) 203,203,505
505 WRITE(IWRIT,5005)
NOXEQ=1
RETURN

C***** CHECK THAT DATA NOT GIVEN BEFORE.

203 IF(ABS(STREM(IDUM,JDUM))-1.0E-6) 61,61,500
500 WRITE(IWRIT,5000) IDUM,JDUM
NOXEQ=1

C***** STORE DATA (-VE FOR SPECIFICATION, +VE FOR
C***** ESTIMATION)

61 STREM(IDUM,JDUM)=RV(I-1)*ISPEC

C***** FCHO CHECK GIVEN STREAM DATA IF DESIRED.

70 IF(IDBUG(14)-2) 803,802,802
802 ILINE=JLINE+1+(NR+2)/3
IF(ILINE-54) 805,805,804
804 WRITE(IWRIT,3333)
3333 FORMAT('1'////)
WRITE(IWRIT,1002)
ILINE=5+(NR+2)/3

SUBROUTINE INPT4 ...(CONT'D)

```

805 CONTINUE
   WRITE(IWRIT,1005) IV(1), (IBRC1, IV(I+1), IBRC2, RV(I), I=1
   $, NR)
   WRITE(IWPIT,1006)
803 CONTINUE
   RETURN
1000 FORMAT(///T36'ECHO CHECK OF STREAM SPECIFICATION DATA'
   $///)
1001 FORMAT(///T37'ECHO CHECK OF STREAM ESTIMATION DATA'//
   $/)
1002 FORMAT(T25'STREAM -           '(PARAMETER NO.)PARAMETER
   $ VALUE'' REPEA
   ITED'//)
1005 FORMAT(T25'-' ,I3,' - ', (' ',T35, A1,I2,A1,E12.5,1X,A1
   $,I2,A1,E12.5,
   11X,A1,I2,A1,E12.5))
1006 FORMAT(' ')
5000 FORMAT('O  STREAM ',I3,'  PARAMETER ',I3,'  MULTIPLY
   $ GIVEN')
5001 FORMAT('O  INCONSISTENT NUMBER OF TOTAL STREAM
   $ PARAMETERS')
5003 FORMAT('O  PARAMETERS AND PARAMETER NO.S DON'T
   $ MATCH')
5004 FORMAT('  INVALID STREAM NUMBER .  (RANGE IS 1 TO
   $ 50)')
5005 FORMAT('  INVALID PARAMETER NUMBER.  (RANGE IS 1 TO
   $ 22)')
5006 FORMAT('O  TOO MANY PAR. GIVEN - (MAX - 20 COMP.+TEMP.
   $+PRESS.)')
5007 FORMAT('O  SPECIFICATION MUST BE DONE BEFORE
   $ ESTIMATION')
      END

```



```

C *****
C *
C *          SUBROUTINE INPT5
C *
C * FUNCTIONS -
C *
C * - FLOWSHEET DATA INPUT ROUTINE
C * - INITIALIZES FLOWSHEET MATRIX (INFO) ELEMENTS TO
C *   ZERO
C * - SETS STREAM UNKNOWN TO 1 IF NOT GIVEN
C * - STORES FLOWSHEET DATA IN INFO AND ECHO CHECKS
C *   IF DESIRED (IDBUG(14)=2 OR GREATER)
C *
C *****

```

```

      SUBROUTINE INPT5(IND)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /INPUT1/IV(25),RV(25),IALPH(50),NI,NR,NA,NOXEQ
      COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM

```

```

C*****      CHECK FOR EXISTENCE OF INTEGER DATA.  IF NONE
C*****      ,RETURN

```

```

      IF(NI) 91,91,90
      91 RETURN

```

```

C*****      CHECK IF DATA INITIALIZATION DONE (IND=1) OR NOT
C*****      (IND=0).

```

```

      90 IF(IND) 100,100,101
      100 IND=1
      NOSTM=0

```

```

C*****      INITIALIZE FLOWSHEET MATRIX, INFO, TO ZERO.

```

```

      DO 1 I=1,50
      DO 1 J=1,5
      1 INFO(I,J)=0

```

```

C*****      INITIALIZE ECHO CHECK IF DESIRED.

```

```

      IF(IDBUG(14)-2) 801,800,800
      800 WRITE(IWRIT,1000)
      801 CONTINUE
      101 NOSTM=NOSTM+1

```

```

C*****      CHECK FOR VALID NUMBER OF INTEGER DATA (3,4 OR 5).

```

```

      IF(NI-5) 94,94,504
      94 IF(NI-3) 504,95,95
      504 WRITE(IWRIT,5004)
      NOXEQ=1

```


SUBROUTINE INPT5 ...(CONT'D)

RETURN

C***** CERTIFY NO REAL DATA.

```
95 IF(NR)500,102,500
500 WRITE(IWPIT,5000)
    NOXEQ=1
102 IDUM=IV(1)
```

C***** CHECK FOR VALID STREAM NUMBER (1-50).

```
    IF(IDUM-50) 120,120,501
120 IF(IDUM)501,501,103
501 WRITE(IWRIT,5001)
    NOXEQ=1
```

C***** CHECK THAT STREAM NOT GIVEN BEFORE.

```
103 IF(INFO(IDUM,1)) 502,104,502
502 WRITE(IWRIT,5002) IDUM
    NOXEQ=1
```

C***** SET STREAM NUMBER.

```
104 INFO(IDUM,1)=IDUM
```

C***** CHECK FOR VALID SOURCE EQUIP. NUMBER. (0 FOR
C***** FEED OR 1-25).

```
    IF(IV(2)-25) 105,105,503
105 IF(IV(2))503,106,106
503 WRITE(IWRIT,5003)
    NOXEQ=1
    RETURN
```

C***** SET SOURCE EQUIP.

```
106 INFO(IDUM,2)=IV(2)
```

C***** CHECK FOR VALID DEST. EQUIP. NO. (0 FOR PROD. OR
C***** 1-25).

```
    IF(IV(3)-25) 107,107,503
107 IF(IV(3)) 503,108,108
```

C***** SET DESTINATION EQUIP.

```
108 INFO(IDUM,3)=IV(3)
    IF(IV(2)-IV(3)) 109,506,109
506 WRITE(IWRIT,5006)
```


SUBROUTINE INPT5 ...(CONT'D)

NOXEQ=1

```

C***** CHECK TO SEE IF 3,4 OR 5 INTEGERS HAVE BEEN GIVEN
C***** . 3 - STRM. NO.,S. EQUIP. AND D. EQUIP. GIVEN
C***** ONLY - GO TO ECHO. 4 - STRM. UNKNOWNNS ALSO GIVEN
C***** . 5 - EVERYTHING GIVEN.
C***** SET STREAM UNKNOWNNS TO 1 IF NOT GIVEN.

```

```

109 INFO(IDUM,4)=1
   IF(NI-4) 200,110,111

```

```

C***** SET STREAM FLAG.

```

```

111 INFO(IDUM,5)=IV(5)

```

```

C***** CHECK FOR VALID STREAM UNKNOWNNS (MUST BE +VE).

```

```

110 IF(IV(4)) 505,112,112
505 WRITE(IWRIT,5005)
   NOXEQ=1

```

```

C***** SET STREAM UNKNOWNNS

```

```

112 INFO(IDUM,4)=IV(4)

```

```

C***** ECHO CHECK IF DESIRED.

```

```

200 IF(IDBUG(14)-2) 803,802,802
802 WRITE(IWRIT,1002) (INFO(IDUM,I),I=1,5)
803 CONTINUE
   RETURN

```

```

1000 FORMAT(///T41'ECHO CHECK OF FLOWSHEET DATA'///T25
$ 'STREAM
1 SOURCE DESTINATION STREAM STREAM'/T25
$, 'N
NUMBER EQUIP. NO. EQUIP. NO. UNKNOWNNS
$ FLAG'///)

```

```

1002 FORMAT(T26,I3,2(12X,I3),10X,I3,8X,I3)
5004 FORMAT('O INVALID NUMBER OF INTEGERS GIVEN. (MUST BE
$ 3,4 OR 5')
5000 FORMAT('O INVALID FLOWSHEET DATA - INTEGERS ONLY')
5001 FORMAT('O INVALID STREAM NUMBER. (RANGE IS 1 TO
$ 50)')
5002 FORMAT('O STREAM ',I3,' GIVEN MORE THAN ONCE')
5003 FORMAT('O INVALID EQUIP. NO. (RANGE IS 0 TO 25)')
5005 FORMAT('O INVALID STREAM UNKNOWNNS - MUST BE ZERO OR
$+VE')
5006 FORMAT('O SELF-LOOPS NOT ALLOWED. ')
END

```



```

C *****
C *
C *          SUBROUTINE FFINP
C *
C *  FUNCTIONS -
C *
C *  -  FREE FORMAT INPUT ROUTINE
C *  -  READS DATA AS FORTRAN ALPHAMERIC INPUT
C *      AND ANALYSES RESULTING ALPHAMERIC VECTOR A
C *      COLUMN AT A TIME
C *  -  STORES INTEGERS, REALS AND ALPHAMERICS IN
C *      APPROPRIATE INPUT VECTORS AS ENCOUNTERED.
C *  -  IGNORES REMAINDER OF CARD IF C ENCOUNTERED
C *      (DATA COMMENT)
C *  -  CODES DATA CONTROL MESSAGES (ENCLOSED IN
C *      ASTERISKS) FOR INPUT ANALYSIS CONTROL
C *  -  FLAGS ERROR IF SYNTAX ERROR ENCOUNTERED
C *
C *****

```

```

SUBROUTINE FFINP(IV,RV,IALPH,NI,NR,NA,ID1,ID2,KFLAG
$,TVALU)
  DIMENSION IV(25),RV(25),IALPH(50),ICODE(19),INPUT(80)
  DATA ICODE/' ','0 ','1 ','2 ','3 ','4 ','5 ','6 ',
1'7 ','8 ','9 ','E ','+ ','- ','.',',*',',',',
1'C '/'
  DATA END,ENDAL/-90624.,-357888./
  DATA IBLNK,ISPAC,ICARD/' ',' ',0/

```

```

C*****      KFLAG - DATA INPUT CONTROL
C*****      = 0  UNSPECIFIED INPUT (CONTINUE)
C*****      = 1  SPECIFIED INPUT (CONTINUE)
C*****      = 2  UNSPECIFIED INPUT (START WITH NEW CARD)
C*****      = 3  SPECIFIED INPUT (START WITH NEW CARD)
C*****      NI,NR,NA      - RELEVANT ONLY FOR KFLAG =1 OR 3.
C*****      NI - SPECIFIED NUMBER OF INTEGERS TO BE READ.
C*****      NR - NUMBER OF REALS TO BE READ.
C*****      NA - NUMBER OF ALPHA-NUMERICS (A1) TO BE READ.
C*****      IICNT - ENCOUNTERED INTEGER COUNTER
C*****      IRCNT - ENCOUNTERED REAL COUNTER
C*****      IACNT - ALPHA-NUMERIC COUNTER
C*****      IRTN - RETURN FLAG (FOR ** CONTROL)
C*****      TVALU - CONTROL MESSAGE CODE.
C*****      ICARD - CARD COUNTER
C*****      IVLD - = 1 IF VALID FIELD EXISTS, 0 OTHERWISE.
C*****      IEXP - = 1 IF EXP ENCOUNTERED IN PRESENT FIELD.
C*****      IDEC - = 1 IF DECIMAL ENC'T'D. IN PRESENT FIELD.
C*****      ICALC - = 1 WHEN FIELD DELIMITED AND STORED.
C*****      ISIGN - = 1 IF SIGN ENC'T'D. IN PRESENT FIELD.
C*****      IMULT =1 FOR POS. , -1 FOR NEG. NUMBER
C*****      IVAL - ACCUMULATED INTEGER VALUE.
C*****      IDCNT - DECIMAL COUNTER FOR ACCUM. REAL NUMBER.

```


SUBROUTINE FFIMP ... (CONT'D)

C***** I - RECORD COLUMN COUNTER.
 C***** INITIALIZE COUNTERS AND FLAGS

IFACT=IBLNK/16448
 IWRT=ID1
 IREAD=ID2
 IICNT=1
 IRCNT=1
 IACNT=1
 ITOT=NI+NR+NA+3
 ITRN=0
 IEND=0

C***** ZERO OUTPUT VECTORS.

DO 10 KKK=1,25
 IV(KKK)=0
 RV(KKK)=0.0
 10 IALPH(KKK)=IBLNK
 TVALU=0.0

C***** INITIALIZE FLAGS

IVLD=0
 IEXP=0
 IVAL=0
 IDEC=0
 ICALC=0
 ISIGN=0
 IDCNT=1
 IMULT=1

C***** IF KFLAG G.E. 2 READ NEW CARD, OTHERWISE CONTINUE
 C***** * WITH LAST RECORD READ.

IF(KFLAG-2) 7,1,1
 7 IF(ICARD) 2,2,105
 1 KFLAG=KFLAG-2
 2 READ(IREAD,1000) INPUT
 ICARD=ICARD+1

C***** HERE TO 105 ANALYZE RECORD ONE COLUMN AT A TIME

I=1
 3 CONTINUE

C***** HERE TO 5 - IDENTIFY COLUMN CHARACTER BY
 C***** SUCCESSIVE COMPARISON WITH CHARACTERS IN CODE
 C***** VECTOR.

SUBROUTINE FEINP ... (CONT'D)

```

DO 5 J=1,19
  IF(ICODE(J)-INPUT(I)) 5,6,5
5 CONTINUE
  GO TO 150

```

```

C*****      BRANCH TO APPROPRIATE SECTION OF PROGRAM ,
C*****      DEPENDING UPON *      CHARACTER FOUND.

```

```

6 GO TO (200,300,300,300,300,300,300,300,300,300,300,300,
1400,500,500,700,800,600,900,199) , J

```

```

C*****      'C ' CHARACTER DETECTED - COMMENT IN DATA - IGNORE
C*****      REMAINDER OF PRESENT CARD.

```

```

199 I=80
  GO TO 105

```

```

C*****      ' ' (BLANK) IGNORE OR TREAT AS DELIMITER,
C*****      DEPENDING UPON THE FIELD STATUS (IVLD).

```

```

200 IF(IVLD) 150,105,210
210 ICALC=1
  GO TO 711

```

```

C*****      '0 ' TO '9 ' (NUMERIC CHARACTER) - MODIFY
C*****      EXISTING ACCUMULATED NUMBER IN FIELD.

```

```

300 IVLD=1
  ICALC=0
  IF(IDECL) 150,301,302
301 IVAL=IVAL*10+(J-2)
  GO TO 105
302 RVAL=RVAL+(J-2.0)/10.0**IDCNT
  IDCNT=IDCNT+1
  GO TO 105

```

```

C*****      'E ' (EXPONENT CHARACTER) - STORE ACCUMULATED
C*****      NUMBER AND PREPARE FOR EVALUATION OF EXPONENT.

```

```

400 IF(IVLD) 150,150,401
401 IF(IEXP) 150,402,150
402 IEXP=1
  IF(IDECL) 150,404,403
403 RV(IRCNT)=RVAL*IMULT
  GO TO 405
404 RV(IRCNT)=IVAL*IMULT
405 IMULT=1
  IVLD=0
  ISIGN=0
  IDECL=0

```


SUBROUTINE FFIMP ... (CONT'D)

```
IVAL=0
GO TO 105
```

```
C*****      '+ ' OR '- ' (SIGN CHARACTER) - SET FLAG.
```

```
500 IF(ISIGN) 150,501,150
501 IF(IVLD) 150,502,150
502 ISIGN=1
    IF(J-13) 150,105,503
503 IMULT=-1
    GO TO 105
```

```
C*****      '* ' (CONTROL CHARACTER) - ANALYZE MESSAGE
C*****      BETWEEN CONTROL CHARACTERS (IF ANY).
```

```
600 I=I+1
    IF(ICODE(17)-INPUT(I)) 601,602,601
```

```
C*****      IF '***' ENCOUNTERED, FORCE RETURN TO CALLING
C*****      PROGRAM. CHECK 'IRTRN' TO SEE IF VALID RETURN.
```

```
602 IF(IRTRN) 150,105,603
603 IF(KFLAG) 604,604,151
604 IEND=1
    IF(IVLD) 150,606,210
606 NR=IRCNT-1
    NI=IICNT-1
    NA=IACNT-1
    RETURN
```

```
C*****      CODE CONTROL MESSAGE FOR CALLING ROUTINE AND THEN
C*****      PRINT.
C*****      RETURN IF CONTROL MESSAGE ALREADY EXISTS.
```

```
601 IF(ABS(TVALU)-1.) 621,621,620
620 I=I-2
    GO TO 603
621 DO 605 K=I,80
    IF(ICODE(17)-INPUT(K)) 605,607,605
605 TVALU=TVALU+(INPUT(K)-IBLNK)/IFACT
    GO TO 150
607 KK=K-1
    IF(ABS(TVALU-END)-ABS(TVALU/1000.)) 609,609,608
608 IF(ABS(TVALU-ENDAL)-ABS(TVALU/1000.)) 609,609,610
609 I=K
    IF(KFLAG) 604,604,134
610 WRITE(IWRIT,1006) (INPUT(J),J=I,KK)
    I=K
    GO TO 130
```


SUBROUTINE FFIMP ... (CONT'D)

C***** ' , ' (DELIMITER) CALCULATE AND STORE PREVIOUS
 C***** FIELD VALUE IF NOT DONE PREVIOUSLY, REINITIALIZE
 C***** FLAGS.

```

700 IF(ICALC) 150,711,712
712 ICALC=0
    GO TO 105
711 IF(IEXP) 150,703,702
702 RV(IRCNT)=RV(IRCNT)*10.0**{IVAL*IMULT}
    IRCNT=IRCNT+1
    GO TO 706
703 IF(IDEC) 150,705,704
704 RV(IRCNT)=RVAL*IMULT
    IRCNT=IRCNT+1
    GO TO 706
705 IV(IICNT)=IVAL*IMULT
    IICNT=IICNT+1
706 IDEC=0
    IEXP=0
    ISIGN=0
    IVAL=0
    IVLD=0
    IMULT=1
    IDCNT=1
    IF(IEND) 150,130,606
  
```

C***** ' . ' (DECIMAL) - FLOAT ACCUMULATED INTEGER.

```

800 IF(IEXP) 150,801,150
801 IF(IDEC) 150,802,150
802 IVLD=1
    IDEC=1
    ICALC=0
    RVAL=IVAL
    GO TO 105
  
```

C***** ' ' ' (QUOTE) STORE DATA BETWEEN QUOTES AS
 C***** ALPHA-NUMERIC DATA.

```

900 I=I+1
    DO 905 K=I,80
        IF(ICODE(18)-INPUT(K)) 904,907,904
904 IALPH(IACNT)=INPUT(K)
905 IACNT=IACNT+1
    GO TO 150
907 I=K
    GO TO 130
105 I=I+1
  
```

C***** CHECK IF END OF RECORD REACHED.

SUBROUTINE FFINP ... (CONT'D)

```
IF(I-80) 3,3,130
```

```
C***** CHECK IF SPECIFIED DATA READ (IF APPLICABLE) ,
```

```
130 ITRN=1
```

```
IF(IVLD) 150,131,210
```

```
131 IF(KFLAG) 150,133,132
```

```
132 IF(ITOT-IICNT-IRCNT-IACNT) 152,134,133
```

```
133 IF(I-80) 105,105,2
```

```
134 IF(NI-IICNT+1) 152,135,152
```

```
135 IF(NR-IRCNT+1) 152,136,152
```

```
136 IF(NA-IACNT+1) 152,137,152
```

```
137 RETURN
```

```
C***** ERROR MESSAGES.
```

```
150 WRITE(IWRIT,1001) ICARD
```

```
GO TO 153
```

```
151 WRITE(IWRIT,1002) ICARD
```

```
GO TO 153
```

```
152 WRITE(IWRIT,1003) ICARD
```

```
153 KFLAG=-1
```

```
GO TO 137
```

```
1000 FORMAT(80A1)
```

```
1001 FORMAT(1H , 'SYNTAX ERROR IN CARD ', I3)
```

```
1002 FORMAT(1H , ' END OF DATA ENCOUNTERED BEFORE SPECIFIED  
$ DATA READ,
```

```
1 '/' (**) , CARD ', I3)
```

```
1003 FORMAT(1H , 'DATA DOES NOT CONFORM TO THAT REQUESTED IN  
$ NUMBER AND/
```

```
1OR TYPE, - CARD NO. ', I3)
```

```
1006 FORMAT(1H0, T25, 80A1)
```

```
END
```



```

C *****
C *
C *          SUBROUTINE SPECL
C *
C *  FUNCTIONS -
C *
C *  - FINAL INPUT DATA CHECKING ROUTINE
C *  - CALLED WHEN DATA INPUT IS FINISHED TO COMPLETE
C *    DATA CHECKING AND DATA STORAGE
C *  - IDENTIFIES ATOM TYPES ( S O C H N ) IN THAT
C *    ORDER IF PRESENT
C *  - REARRANGES STREAM DATA TO CORRESPOND WITH
C *    REARRANGED M AND T DATA (I.E. LIQUID SPECIES
C *    STORED LAST)
C *  - CHECKS VALIDITY OF INFORMATION STREAMS
C *    (INFORMATION DESTINATIONS)
C *
C *****

```

```

SUBROUTINE SPECL
  DIMENSION IDVEC(5),SSTOR(20),IVALD(5,5)
  COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
  COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)
  COMMON /EXEC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
  $,ISUPR,IOP
  COMMON /STOR1/EQUIP(300),ILOP,NMREQ,STREM(50,22)
  $,NSIN(5),NSOUT(5)
  COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
  COMMON /INPUT1/IV(25),RV(25),IALPH(50),NI,NR,NA,NOXEQ
  COMMON /INPUT2/ISYMB(20),IATOM(5),ATMWT(5),VATOM(5)
  $,KEQIV(20)
  DATA IDVEC/'S','O','C','H','N'/
  DATA IVALD/1,6,0,0,0,19,1,0,0,0,21,0,0,0,0,23,0,0,0,0
  $,0,0,0,0,0/

```

```

C*****      IDENTIFY ATOM TYPES IN ORDER S O C H N, IF PRESENT
C*****      AND STORE LOCATIONS IN IDATM.

```

```

      DO 1 I=1,5
      DO 2 J=1,5
      IF(IATOM(I)-IDVEC(J)) 2,3,2
3 IDATM(J)=I
      GO TO 1
2 CONTINUE
1 CONTINUE

```

```

C*****      REARRANGE COMPONENTS IN STREAM DATA IF LIQUID
C*****      SPECIES WERE NOT READ IN LAST.

```

```

      DO 5 I=1,NGMS
      IF(KEQIV(I)-I) 6,5,6
5 CONTINUE

```


SUBROUTINE SPFCL ... (CONT'D)

```

      GO TO 900
      6 DO 10 I=1,50

```

```

C*****      CHECK THAT STREAM EXISTS AND IS NOT INFORMATION
C*****      STREAM.

```

```

      IF( INFO(I,1)) 10,10,11
11 IF( INFO(I,5)) 10,12,12
12 DO 13 J=1,NTOT
13 SSTOR(J)=STREM(I,J)

```

```

C*****      RESTORE STREAM COMPONENTS IN CORRECT ORDER.

```

```

      DO 14 J=1,NTOT
      IJ=KEQIV(J)
14 STREM(I,J)=SSTOR(IJ)
10 CONTINUE
900 CONTINUE

```

```

C*****      CHECK VALIDITY OF INFO STREAM INFO DESTINATION.

```

```

      IF(NOSTM) 902,902,901
901 DO 100 I=1,50
      IF( INFO(I,5)) 50,100,100
      50 NSTRM=INFO(I,1)
      NETO=INFO(I,3)
      NTYPE=JTYPE(NETO)
      DO 60 J=1,5
      IF(NTYPE-IVALD(J,1)) 60,55,60
      55 NNN=J
      GO TO 61
      60 CONTINUE
      WRITE(IWRIT,3000) NSTRM,NETO,NTYPE
      NOXEQ=1
      GO TO 100
      61 DO 70 K=1,5,2
      NPAR=ABS(STREM(NSTRM,K))+0.5
      DO 65 J=2,5
      IF(NPAR-IVALD(NNN,J)) 65,69,65
      65 CONTINUE
      WRITE(IWRIT,3001) NSTRM, NPAR,NTYPE
      NOXEQ=1
      GO TO 100
      69 IF(NPAR) 70,70,71
      71 ILOC=INDEX(NETO)
      CALL COMPR(NSTRM,K+1,NPAR)
      70 CONTINUE
      100 CONTINUE
      902 RETURN
3000 FORMAT('O INFO. STREAM 'I3' TO EQUIP. NO.'I3' IS IN

```


SUBROUTINE SPECL ... (CONT'D)

```
$ ERROR'/  
1' EQUIP. TYPE 'I3' WILL NOT SUPPORT INFO. INPUT.')
```

3001 FORMAT('O INFO. STREAM 'I3' IS IN ERROR, PAR. NO. 'I2
\$/
1' IS NOT A VALID INFO INPUT TO EQUIP. TYPE 'I3)
END


```

C *****
C *
C *          SUBROUTINE OPTIM
C *
C * FUNCTIONS -
C *
C * - CALCULATION SEQUENCE OPTIMIZATION EXECUTIVE
C * - INITIALIZES 'INFO' MATRIX FOR OPTIMIZATION
C *   (MASKS PLANT FEEDS AND PRODUCTS AND SERVICE
C *   STREAMS)
C * - REDUCES THE FLOWSHEET -- TERMINATES THE
C *   OPTIMIZATION IF THE FLOWSHEET HAS BEEN
C *   COMPLETELY REDUCED
C * - OPTIMIZES THE ORDER OF CALCULATIONS
C * - RESTORES THE 'INFO' MATRIX WHEN OPTIMIZATION
C *   IS COMPLETE
C *
C *****

```

SUBROUTINE OPTIM

```

C***** THIS ROUTINE CONTROLS THE SEARCHING FOR THE OPTIMAL
C***** CALCULATION SEQUENCE. THE CRITERION OF OPTIMALITY
C***** IS THAT THE NUMBER OF RECYCLE PARAMETERS GUESSED
C***** BE A MINIMUM.
C*****

```

```

COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /EXEC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
$,ISUPR,IOPT
COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
COMMON /OPT1/IDELT(26,26),IREC(25),NDEQP,NP1,ISIGM

```

```

C***** INITIALIZE INFO MATRIX FOR OPTIMIZATION.
C***** (NEGATE STREAM NUMBERS OF ALL PLANT FEEDS (INFO(-
C***** ,2)=0), PLANT PRODUCTS (INFO(-,3)=0) AND SERVICE
C***** STREAMS (INFO(-,5) +VE), SO THEY WILL BE IGNORED
C***** IN THE OPTIMIZATION.)

```

```

DO 3 I=1,50
  IF(INFO(I,5)) 1,1,2
1 IF(INFO(I,2)*INFO(I,3)) 3,2,3
2 INFO(I,1)=-INFO(I,1)
3 CONTINUE

```

```

C***** CALL 'REDUC' TO ATTEMPT TO SIMPLIFY FLOWSHEET FOR
C***** OPTIMIZATION PURPOSES.

```

```

CALL REDUC

```

```

C***** IF FLOWSHEET COMPLETELY REDUCED, TERMINATE.

```


SUBROUTINE OPTIM ... (CONT'D)

```

      IF(NOEQP-1) 10,10,20
10  CALL SEQNC
      GO TO 999

```

```

C*****  CALL 'DELTA'  TO INITIALIZE 'IDELT' MATRIX FROM
C*****  SIMPLIFIED FLOWSHEET

```

```

      20 CALL DELTA

```

```

C*****  INITIALIZE NUMB  - STEP COUNTER

```

```

      NUMB=0

```

```

C*****  CALL 'DCHCK'  TO FIND ANY POSSIBLE SEQUENCE
C*****  IMPROVEMENT

```

```

      100 CALL DCHCK(II,JJ,IFLAG)

```

```

C*****  CALL 'FINSH'  TO DETERMINE NEXT MOVE

```

```

      CALL FINSH (IFLAG,JFLAG)

```

```

C*****          JFLAG=0  SEQUENCE RANDOMIZED, SKIP TO DCHCK
C*****          JFLAG=1  CONTINUE WITH NEXT STEP
C*****          JFLAG=2  OPTIMIZATION COMPLETE, TERMINATE

```

```

      IF(JFLAG-1) 100,300,999

```

```

C*****  CALL 'EXCHN'  TO AFFECT BENEFICIAL MOVE FOUND BY
C*****  'DCHCK'

```

```

      300 CALL EXCHN (II,JJ,IFLAG)
      NUMB=NUMB+1
      GO TO 100
      999 CONTINUE

```

```

C*****  RETURN INFO MATRIX TO ORIGINAL FORM.

```

```

      DO 500 I=1,50
      IF(INFO(I,1)) 499,500,500
499  INFO(I,1)=-INFO(I,1)
500  CONTINUE
      WRITE(IWRIT,2000) (ISEQ(I),I=1,NNEQP)
      KASUM=0
      DO 501 I=1,25
      IF(IASUM(I)) 502,502,501
501  KASUM=KASUM+1
502  IF(KASUM) 505,505,504
504  WRITE(IWRIT,2001) (IASUM(I),I=1,KASUM)
      GO TO 506

```


SUBROUTINE OPTIM ... (CONT'D)

```
505 WRITE(IWRIT,2003)
506 CONTINUE
    WRITE(IWRIT,9000)
    RETURN
2000 FORMAT('0'T35'THE OPTIMIZED CALCULATION SEQUENCE IS -'
    $/
    1(/T25,20I3))
2001 FORMAT('0'T35'THE FOLLOWING STREAMS MUST BE ASSUMED,'/
    1(/T40,10I3))
2003 FORMAT('0'T42'NO STREAMS NEED BE ASSUMED')
9000 FORMAT('0',T25,'*****')
    $*****
    1*****')/
    END
```



```

C *****
C *
C *          SUBROUTINE REDUC
C *
C * FUNCTIONS -
C *
C * - FLOWSHEET SIMPLIFICATION ROUTINE
C * - ATTEMPTS TO REDUCE THE COMPLEXITY OF THE
C *   FLOWSHEET (AND OPTIMIZATION) IN TWO PHASES
C * - STORES ELIMINATED EQUIPMENT IN FINAL SEQUENCE
C *   VECTOR (PHASE 1) OR SAVES LINKS (PHASE 2) SO
C *   FINAL SEQUENCE CAN BE OBTAINED FROM OPTIMIZED
C *   REDUCED SEQUENCE WHEN OPTIMIZATION IS COMPLETE
C *
C *****

```

SUBROUTINE REDUC

```

C*****  THIS SUBROUTINE ATTEMPTS TO SIMPLIFY THE FLOWSHEET
C*****  GIVEN, IN ORDER TO EASE THE SEARCH FOR THE OPTIMUM
C*****  CALCULATION SEQUENCE. THIS IS DONE IN TWO PHASES.
C*****
C*****  (1) ELIMINATION OF ALL EQUIP. WITH NO
C*****  ANTICEDENTS (PLACE AT FRONT OF 'ISEQ',
C*****  KTOP INCREMENTED) AND ELIMINATION OF ALL
C*****  EQUIP. WITH NO DECENDANTS (PLACED AT BACK
C*****  OF 'ISEQ', KBOT DECREMENTED). KFLAG=0 FOR
C*****  PHASE ONE
C*****  (2) ELIMINATION OF EQUIP. WITH SINGLE
C*****  INPUT & SINGLE OUTPUT. ELIMINATION IS
C*****  ACCOMPANIED BY INTRODUCTION OF
C*****  PSEUDO-STREAM, NEGATION OF STREAMS
C*****  INVOLVING THE ELIMINATED EQUIP. AND
C*****  STORAGE OF SEQUENTIAL LINKS IN MATRIX
C*****  'ILINK'
C*****  ONE OF THE FOLLOWING SETS OF CONDITIONS
C*****  MUST BE MET BESIDES THE ONE ABOVE BEFORE
C*****  EQUIP. ELIMINATION RESULTS. PHASE 2-A IS
C*****  FINISHED BEFORE PHASE 2-B BEGINS
C*****  (2)(A)-DENOTE EQUIP. SUPPLYING THE SINGLE
C*****  INPUT TO THE ELIMINATED EQUIP. AS SOURCE
C*****  THEN SOURCE MUST ALSO HAVE A SINGLE INPUT
C*****  , AND THE NUMBER OF STREAM UNKNOWNNS
C*****  (INFO(-,4)) OF THE ELIMINATED EQUIP. MUST
C*****  BE EQUAL OR GREATER THAN INFO(-,4) FOR
C*****  THE SOURCE INPUT. KFLAG=1 FOR PHASE 2-A
C*****  (2)(B)-DENOTE THE EQUIP. DESTINATION OF
C*****  THE SINGLE OUTPUT OF THE ELIMINATED
C*****  EQUIP. AS DEST. THEN DEST MUST HAVE A
C*****  SINGLE INPUT AND THE NUMBER OF STREAM
C*****  UNKNOWNNS (INFO(-,4)) OF THE ELIMINATED
C*****  EQUIP INPUT MUST BE EQUAL TO OR LESS THAN
C*****  THE NUMBER FOR THE OUTPUT (INPUT TO

```


SUBROUTINE REDUC ... (CONT'D)

```

C*****      DEST). KFLAG=2 FOR PHASE 2-B
C*****
C*****      'IREC'      SIMPLIFIED FLOWSHEET SEQUENCE VECTOR
C*****      'ISEQ'      TOTAL FLOWSHEET SEQUENCE VECTOR

      DIMENSION INOUT(3,25),IFLIM(25)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /EXEC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
      $,ISUPR,IQPT
      COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
      COMMON /OPT1/IDELT(26,26),IREC(25),NOEQP,NP1,ISIGM
      COMMON /OPT2/ILINK(25,2),LOCAL(25),KSUDO,KTOP,KBOT
      DATA IA,IB/'A','B'/

C*****      INITIALIZE PARAMETERS AND FLAGS.

      KSUDO=50
      NOEQP=NNEQP
      NP1=NOEQP+1
      ISIGM=999

C*****      INITIALIZE SEQUENCE VECTOR FROM GIVEN SEQUENCE.

      DO 1234 I=1,NNEQP
1234  IREC(I)=ISEQ(I)

C*****      INITIALIZE PHASE INDICATOR (KFLAG), SEQ. LINK
C*****      COUNTER (KLINK), AND ELIMINATED EQUIP. COUNTER
C*****      (IFLIM).

      KFLAG=0
      KLINK=1
      KELIM=0

C*****      WRITE OUT THE INITIAL SEQUENCE

      WRITE(IWRIT,2049)
      WRITE(IWRIT,9000)
      WRITE(IWRIT,2050) (IREC(I),I=1,NNEQP)
      WRITE(IWRIT,2051)

C*****      INITIALIZE 'ISEQ' LOCATION COUNTERS

      KTOP=1
      KBOT=NNEQP

C*****      HERE TO 14      INITIALIZE 'ISEQ' & SEQ. LINK MATRIX
C*****      'ILINK'

      DO 14 I=1,25

```


SUBROUTINE REDUC ... (CONT'D)

```

      ISEQ(I)=0
      ILINK(I,1)=0
14  ILINK(I,2)=0
201 CONTINUE

```

```

C*****  HERE TO 1 BUILD 'LOCAL' VECTOR AND INITIALIZE
C*****  'INOUT' MATRIX.
C*****  LOCAL(I) CONTAINS 'IREC' LOCATION
C*****  (1-NDEQP) OF EQUIP. NO 'I'

```

```

      DO 1 K=1,NDEQP
      LDUM=IABS(IREC(K))
      IF(LDUM) 70,1,70
70  LOCAL(LDUM)=K
      INOUT(1,LDUM)=0
      INOUT(2,LDUM)=0
1  CONTINUE

```

```

C*****  HERE TO 2 BUILD 'INOUT' MATRIX FROM FLOWSHEET DATA
C          'INFO' , SUCH THAT-
C*****  INOUT(1,I)=0   IF NO INPUTS TO EQUIP I
C*****  = +VE IF ONE INPUT TO I
C*****  (=SOURCE EQUIP.)
C*****  = -VE IF MORE THAN ONE INPUT
C*****  TO EQUIP I
C*****  INOUT(2,I)=0   IF NO OUTPUT FROM EQUIP I
C*****  = +VE IF ONE OUTPUT FROM I
C*****  (= DESTINATION)
C*****  = -VE IF MORE THAN ONE OUTPUT
C*****  FROM EQUIP I
C*****  INOUT(3,I)= NUMBER OF STREAM ASSUMPTIONS
C*****  ASSOCIATED WITH LAST INPUT TO
C*****  I ENCOUNTERED
C*****  NOTE-  SYSTEM FEEDS AND PRODUCTS ARE IGNORED
C*****  ABOVE.  FEEDS ARE ASSUMED KNOWN

```

```

      DO 2 K=1,KSUDO
      IF(INFO(K,1))2,2,3
3  IINP=INFO(K,3)
      IOUT=INFO(K,2)
      IF(INOUT(1,IINP))4,5,5
5  INOUT(1,IINP)=IOUT-100*INOUT(1,IINP)
      INOUT(3,IINP)=INFO(K,4)
4  IF(INOUT(2,IOUT))2,6,6
6  INOUT(2,IOUT)=IINP-100*INOUT(2,IOUT)
2  CONTINUE

```

```

C*****  JUMP TO 7 (PHASE 1,KFLAG=0) OR 8 (PHASE 2,KFLAG=1
C*****  OR 2)

```


SUBROUTINE REDUC ... (CONT'D)

IF(KFLAG) 7,7,8
7 CONTINUE

C***** HERE TO 9 ELIMINATE EQUIP. WITH NO DECENDANTS
C***** AND/OR NO ANTICEDENTS.
C***** NO ANTICEDENTS TO I INDICATED BY INOUT(1,I)=0
C***** NO DECENDENTS FROM I INDICATED BY INOUT(2,I)=0

DO 9 I=1,NDEQP

C***** IF IREC(I) ZERO, THAT LOCATION ALREADY ELIMINATED
C***** - IGNORE

IF(IREC(I)) 10,9,10
10 IEQP=IABS(IREC(I))
IF(INOUT(1,IEQP)) 11,12,11

C***** STORE IN 'ISEQ' AND ELIMINATE EQUIP IN 'IREC'

12 ISEQ(KTOP)=IEQP
KTOP=KTOP+1
IREC(I)=0
IF(IDBUG(13)-2) 803,802,802
802 WRITE(IWRIT,2000) IEQP
803 CONTINUE

C***** ELIMINATE EQUIP. STREAMS (AT 100) AND BEGIN NEW
C***** SWEEP

GO TO 100
11 IF(INOUT(2,IEQP)) 9,13,9

C***** STORE IN 'ISEQ' AND ELIMINATE EQUIP IN 'IREC'

13 ISEQ(KBOT)=IEQP
KBOT=KBOT-1
IREC(I)=0
IF(IDBUG(13)-2) 805,804,804
804 WRITE(IWRIT,2001) IEQP
805 CONTINUE

C***** ELIMINATE EQUIP. STREAMS (AT 100) AND BEGIN NEW
C***** SWEEP

GO TO 100
9 CONTINUE

C***** IF DO LOOP COMPLETED, PHASE ONE FINISHED- SET
C***** KFLAG=1 AND BEGIN PHASE 2

SUBROUTINE REDUC ... (CONT'D)

KFLAG=1
8 CONTINUE

C***** HERE TO 15 ELIMINATE EQUIP. WITH SINGLE INPUT
C***** AND SINGLE OUTPUT.
C***** KEQP IS THE EQUIP WHOSE INPUT UNKNOWNNS ARE TO BE
C***** COMPARED WITH THOSE OF THE ELIMINATED EQUIP.'S
C***** (IEQP)
C***** JEQP IS THE EQUIP BEFORE (PHASE 2-A) OR AFTER
C***** (PHASE 2-B) THE ELIMINATED EQUIP (JEQP WILL BE
C***** NEGATED IN 'IREC' AND STORED IN 'ILINK' IF IEQP IS
C***** ELIMINATED)

DO 15 I=1,NOEQP

C***** IF IREC(I) ZERO, THAT LOCATION ALREADY ELIMINATED
C***** - IGNORE

IF(IREC(I)) 16,15,16
16 IEQP=IABS(IREC(I))

C***** CHECK FOR ONE INPUT & ONE OUTPUT (INOUT(1,I)
C***** ,INOUT(2,I)= +VE)

IF(INOUT(1,IEQP)) 15,15,26
26 IF(INOUT(2,IEQP)) 15,15,27

C***** CHECK FOR GENERATION OF SELF LOOP.

27 IF(INOUT(1,IEQP)-INOUT(2,IEQP)) 17,15,17

C***** JUMP TO 18 (PHASE 2-A,KFLAG=1) OR 19 (PHASE 2-B
C***** ,KFLAG=2)

17 IF(KFLAG-1) 18,18,19

C***** CHECK THAT SOURCE EQUIPMENT ALSO HAS SINGLE INPUT
C***** AND THAT SOURCE INPUT UNKNOWNNS LESS THAN OR EQUAL
C***** TO ELIMINATED INPUT UNKNOWNNS. (IF NOT DO NOT
C***** ELIMINATE IEQP)

18 IPHAS=IA
JEQP=INOUT(1,IEQP)
KEQP=INOUT(2,IEQP)
IF(INOUT(1,JEQP)) 15,15,20
20 IF(INOUT(3,JEQP)-INOUT(3,IEQP)) 21,21,15

C***** CHECK THAT DESTINATION EQUIP. ALSO HAS SINGLE INPUT
C***** & THAT DESTINATION INPUT UNKNOWNNS GREATER THAN OR
C***** EQUAL TO ELIMINATED INPUT UNKNOWNNS (IF NOT DO NOT

SUBROUTINE REDUC ... (CONT'D)

C***** ELIMINATE IEQP)

19 IPHAS=I3

JEQP=INOUT(2,IEQP)

KEQP=IEQP

IF(INOUT(1,JEQP)) 15,15,22

22 IF(INOUT(3,IEQP)-INOUT(3,JEQP)) 21,21,15

C***** IF A SET OF THE ABOVE CONTITIONS IS MET, ELIMINATE
C***** IEQP, CREATE PSEUDO STREAM TO BRIDGE ELIMINATED
C***** EQUIP. AND STORE EQUIP. SEQUENCE LINKS ('ILINKS')-
C***** NEGATE 'IREC' ENTRY TO INDICATE EXISTENCE OF LINKS.

21 IREC(I)=0

IDUM=LOCAL(JEQP)

IREC(IDUM)=-JEQP

KSUDO=KSUDO+1

INFO(KSUDO,1)=KSUDO

INFO(KSUDO,2)=INOUT(1,IEQP)

INFO(KSUDO,3)=INOUT(2,IEQP)

INFO(KSUDO,4)=INOUT(3,KEQP)

IF(KFLAG-1) 23,23,24

C***** PHASE 2-A ELIMINATED EQUIP (IEQP) - RHS 'ILINK'
C***** 'IREC' ENTRY (TO BE NEGATED IN 'IREC') (JEQP) - LHS
C***** 'ILINK')

23 ILINK(KLINK,1)=JEQP

ILINK(KLINK,2)=IEQP

GO TO 25

C***** PHASE 2-B ELIMINATED EQUIP (IEQP) - LHS 'ILINK'
C***** 'IREC' ENTRY (TO BE NEGATED IN 'IREC') (JEQP) - RHS
C***** 'ILINK')

24 ILINK(KLINK,1)=IEQP

ILINK(KLINK,2)=JEQP

C***** INCREMENT LINK COUNTER KLINK

25 KLINK=KLINK+1

IF(IDBUG(13)-2) 807,806,806

806 WRITE(IWRIT,2003) IPHAS,IEQP,JEQP,IFQP,(INFO(KSUDO,II)
\$,II=1,4)

807 CONTINUE

GO TO 100

15 CONTINUE

C***** IF DO LOOP COMPLETED, MEANS FINISHED PHASE 2-A OR
C***** 2-B. INCREMENT KFLAG- IF 2 CONTINUE WITH PHASE

SUBROUTINE REDUC ... (CONT'D)

C***** 2-B... IF 3 TERMINATE REDUCTION, PRINT AND EXIT

KFLAG=KFLAG+1

IF(KFLAG-2) 201,201,202

C***** HERE TO 205 COMPACT 'IREC' BY SQUEEZING OUT ZEROS
C***** RESULTING IN ELIMINATED EQUIP. LOCATIONS

202 KOUNT=1

DO 205 I=1,NOEQP

IF(IREC(I)) 204,205,204

204 ISTORE=IREC(I)

IREC(I)=0

IREC(KOUNT)=ISTORE

KOUNT=KOUNT+1

205 CONTINUE

C***** REDEFINE NOEQP- NO. OF EQUIP.'S IN SIMPLIFIED
C***** FLOWSHEET (NO. OF NON-ZERO ENTRIES IN 'IREC')

NOEQP=KOUNT-1

NP1=NOEQP+1

IF(IDBUG(13)-1) 809,808,808

C***** IF ANY EQUIP. NO.'S HAVE BEEN ELIMINATED BY THE TWO
C***** PHASE REDUCTION, PRINT THEM

808 IF(KELIM) 999,999,206

206 WRITE(IWRIT,2100) (IELIM(I),I=1,KELIM)

809 CONTINUE

IF(IDBUG(13)-2) 811,810,810

810 III=KLINK-1

WRITE(IWRIT,2010) (ILINK(II,1),II=1,III)

WRITE(IWRIT,2011) (ILINK(II,2),II=1,III)

WRITE(IWRIT,2012) (IREC(II),II=1,NOEQP)

WRITE(IWPIT,2051)

811 CONTINUE

999 CONTINUE

RETURN

100 CONTINUE

C***** HERE TO 101 TEMPORARILY ELIMINATE ALL STREAMS
C***** CONTAINING IEQP AS A SOURCE OR DESTINATION IN
C***** FLOWSHEET DATA ('INFO') BY NEGATING THE STREAM
C***** NUMBER(S)

DO 101 I=1,KSUDO

IF(INFO(I,1)) 101,101,104

104 IF(INFO(I,2)-IEQP) 102,103,102

102 IF(INFO(I,3)-IEQP) 101,103,101

SUBROUTINE REDUC ... (CONT'D)

```
103 INFO(I,1)=-INFO(I,1)
```

```
101 CONTINUE
```

```
KELIM=KELIM+1
```

```
C***** STORE ELIMINATED EQUIPMENT NUMBER FOR REDUCTION
```

```
C***** SUMMARY PRINT
```

```
IELIM(KELIM)=IEQP
```

```
GO TO 201
```

```
2000 FORMAT(T25,'PHASE 1, EQUIP. NO. 'I2' HAS NO
```

```
$ ANTICEDENTS - ELIMINAT
```

```
IED.')
```

```
2001 FORMAT(T25,'PHASE 1, EQUIP. NO. 'I2' HAS NO DECENDENTS
```

```
$- ELIMINATED
```

```
1.')
```

```
2003 FORMAT(T25,'PHASE 2-'A1' , EQUIP. NO. 'I2' AND 'I2'
```

```
$ COMBINED, 'I2'
```

```
IELIMINATED, '/T25'PSEUDO-STREAM INTRODUCED -'4I3)
```

```
2010 FORMAT(T25'L.H.S. ILINK MATRIX'/(T25,20I3))
```

```
2011 FORMAT(T25'R.H.S. ILINK MATRIX'/(T25,20I3))
```

```
2012 FORMAT(T25'REDUCED SEQUENCE -'/(T25,20I3))
```

```
2049 FORMAT('1'///// T38'CALCULATION SEQUENCE OPTIMIZATION')
```

```
2050 FORMAT(T44'INITIAL SEQUENCE IS -'/(T25,20I3))
```

```
2051 FORMAT('0')
```

```
2100 FORMAT(/T25'THE FOLLOWING EQUIPMENT NUMBERS ARE
```

```
$ CONSIDERED IRRELE
```

```
1VANT' /T25'WITH RESPECT TO THE OPTIMAL SEQUENCE AND SO
```

```
$ HAVE BEEN' /
```

```
1T25'ELIMINATED WITH APPROPRIATE INTRODUCTION OF PSEUDO
```

```
$ STREAMS -' /
```

```
1(/T25,20I3))
```

```
9000 FORMAT('0',T25,'*****')
```

```
$*****
```

```
1*****')
```

```
END
```



```

C *****
C *
C *          SUBROUTINE DELTA
C *
C *  FUNCTIONS -
C *
C *  -  ASSOCIATION MATRIX UTILITY ROUTINE
C *  -  GENERATES THE 'IDELT' OR ASSOCIATION MATRIX
C *      FOR A GIVEN CALCULATION SEQUENCE USING THE
C *      FLOWSHEET DATA IN 'INFO' MATRIX
C *
C *****

```

SUBROUTINE DELTA

```

C*****  THIS SUBROUTINE , GIVEN THE 'INFO' MATRIX OF
C*****  FLOWSHEET DATA AND A GIVEN SEQUENCE, 'IREC',
C*****  CONSTRUCTS THE 'IDELT' MATRIX USED IN THE SEARCH
C*****  FOR THE OPTIMAL CALCUTIONAL SEQUENCE.
C*****

```

```

COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
COMMON /OPT1/IDELT(26,26),IREC(25),NOEQP,NP1,ISIGM
COMMON /OPT2/ILINK(25,2),LOCAL(25),KSUDO,KTOP,KBOT

```

```

C*****  HERE TO 2 CONSTRUCT 'LOCAL' VECTOR SUCH THAT
C*****  LOCAL(I) IS THE 'IREC' LOCATION OF EQUIP I

```

```

      DO 2 K=1,NOEQP
        LDUM=IABS(IREC(K))
      2  LOCAL(LDUM)=K

```

```

C*****  HERE TO 6 INITIALIZE 'IDELT' MATRIX TO ZERO

```

```

      DO 6 I=1,NP1
        DO 6 J=1,NP1
      6  IDELT(I,J)=0

```

```

C*****  HERE TO 3 CONSTRUCT 'IDELT' MATRIX USING THE
C*****  FLOWSHEET DATA 'INFO' (INCLUDING PSEUDO-STREAMS IF
C*****  ANY) AND THE SEQUENCE 'IREC'

```

```

      DO 3 KSTRM=1,KSUDO

```

```

C*****  IF STREAM NUMBER ZERO OR -VF , IGNORE THAT STREAM

```

```

      IF(INFO(KSTRM,1))3,3,8

```

```

C*****  PLACE NUMBER OF STREAM UNKNOWNNS (INFO(KSTRM,4)) IN
C*****  APPROPRIATE LOCATION IN 'IDELT' (STREAM FROM
C*****  EQUIP. NO. I TO NO. J IS REPRESENTED IN LOCATION
C*****  IDELT(K,L), WHERE IREC(K)=I AND IREC(L)=J

```


SUBROUTINE DELTA ... (CONT'D)

```
8 IDUM=INFO(KSTRM,3)
  JDUM=INFO(KSTRM,2)
  IDUM=LOCAL(IDUM)
  JDUM=LOCAL(JDUM)
  IDELT(IDUM,JDUM)=IDELT(IDUM,JDUM)+INFO(KSTRM,4)
3 CONTINUE
```

```
C***** HERE TO 5 EQUATE LAST ROW & COL. OF 'IDELT' TO
C***** 'IREC' AND MAKE UPPER TRIANGULAR 'IDELT' EQUAL TO
C***** ITSELF MINUS THE LOWER TRIANGULAR 'IDELT'
```

```
DO 5 I=1,NDEQP
  IDELT(I,NP1)=IREC(I)
  IDELT(NP1,I)=IREC(I)
DO 5 J=I,NDEQP
  IDELT(I,J)=IDELT(I,J)-IDELT(J,I)
5 CONTINUE
```

```
C***** RECYCLE APPEARS AS POSITIVE ENTRY IN UPPER
C***** TRIANGULAR 'IDELT', NON-RECYCLE STREAMS AS -VE
C***** ENTRY IN UPPER 'IDELT'
```

```
RETURN
END
```



```

C *****
C *
C *          SUBROUTINE EXCHN
C *
C *  FUNCTIONS -
C *
C *  - SEQUENCE MODIFICATION UTILITY ROUTINE
C *  - ALTERS THE CALCULATION SEQUENCE AND THE
C *    ASSOCIATION MATRIX 'IDELT' IN THE MANNER
C *    DETECTED AS BEING ADVANTAGEOUS BY DCHCK
C *  - ALTERATION IS DONE DIRECTLY FOR SEQUENCE
C *    EXCHANGE OR BY CALLING DELTA FOR SEQUENCE
C *    PROMOTION OR DEMOTION
C *
C *****

```

SUBROUTINE EXCHN(II,JJ,IFLAG)

```

C*****  THIS SUBROUTINE CHANGES THE CALCULATION SEQUENCE
C*****  'IREC' AND THE 'IDELT' MATRIX (DIRECTLY OR BY
C*****  CALLING DELTA) IN THE MANNER DETECTED AS BEING
C*****  ADVANTAGEOUS BY DCHCK
C*****          IFLAG= 1          DEMOTION OF II TO JJ
C*****              = 2          PROMOTION OF JJ TO II
C*****              = 3 OR 4     EXCHANGE OF II & JJ
C*****

```

```

COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /OPT1/IDELT(26,26),IREC(25),NOEQP,NP1,ISIGM
IF(IDBUG(13)-3) 804,800,800
800 IF(IFLAG-2) 801,802,803
801 WRITE(IWRIT,1000) II,JJ,IREC(II)
GO TO 804
802 WRITE(IWRIT,1001) JJ,II,IREC(JJ)
GO TO 804
803 WRITE(IWRIT,1002) II,JJ,IREC(II),IREC(JJ)
804 CONTINUE

```

```

C*****  DECIDE ON MOVE TO BE EXECUTED, DEPENDING UPON
C*****  IFLAG.

```

```

IF(IFLAG-2) 5,7,4

```

```

C*****  HERE TO 2 IFLAG= 3 OR 4
C*****  EXCHANGE POSITION II IN 'IREC' WITH THAT OF JJ
C*****  MODIFY 'IDELT' ACCORDINGLY
C*****  HERE TO 3 CONSTRUCT LOWER 'IDELT' AS -VE MIRROR
C*****  IMAGE OF UPPER TRIANGULAR 'IDELT'

```

```

4 DO 3 I=2,NOEQP
IM1=I-1
DO 3 J=1,IM1

```


SUBROUTINE EXCHN ... (CONT'D)

```

      IDELT(I,J)=-IDELT(J,I)
3  CONTINUE

```

```

C*****  HERE TO 1 EXCHANGE COLUMNS II AND JJ

```

```

      DO 1 I=1,NP1
      ISTORE=IDELT(I,II)
      IDELT(I,II)=IDELT(I,JJ)
      IDELT(I,JJ)=ISTORE
1  CONTINUE

```

```

C*****  HERE TO 2 EXCHANGE ROWS II AND JJ

```

```

      DO 2 J=1,NP1
      ISTORE=IDELT(II,J)
      IDELT(II,J)=IDELT(JJ,J)
      IDELT(JJ,J)=ISTORE
2  CONTINUE

```

```

C*****  TO 203 REDEFINE 'IREC'

```

```

      DO 203 I=1,NDEQP
203  IREC(I)=IDELT(NP1,I)
      GO TO 205

```

```

C*****  IFLAG= 1 , DEMOTE EQUIP NO. IN POSITION II TO
C*****  POSITION JJ
C*****  SHIFT POSITIONS II+1 TO JJ ONE TO LEFT

```

```

5  JJM1=JJ-1
   ISTORE=IREC(II)
   DO 6 I=II,JJM1
6  IREC(I)=IREC(I+1)
   IREC(JJ)=ISTORE
   GO TO 10

```

```

C*****  IFLAG= 2 PROMOTE EQUIP. NO. IN POSITION JJ TO
C*****  POSITION II
C*****  SHIFT POSITIONS II TO JJ-1 ONE TO RIGHT

```

```

7  JJMII=JJ-II
   ISTORE=IREC(JJ)
   DO 8 I=1,JJMII
   IDUM=JJ+1-I
8  IREC(IDUM)=IREC(IDUM-1)
   IREC(II)=ISTORE

```

```

C*****  CALL DELTA TO CONSTRUCT NEW 'IDELT' MATRIX

```

```

10 CALL DELTA

```


SUBROUTINE EXCHN ...(CONT'D)

C***** COMPUTE ISIGM= SUM OF UPPER TRIANGULAR 'IDELT' -
C***** SHOULD BE MINIMUMIZED FOR OPTIMUM SEQUENCE IE. MIN.
C***** RECYCLE ASSUMPTIONS

```
205 ISIGM=0
    DO 202 I=1,NOEQP
    DO 202 J=I,NOEQP
202 ISIGM=ISIGM+IDELT(I,J)
    RETURN
1000 FORMAT(T25'DEMOTE SEQUENCE POSITION'I3' TO'I3' (EQUIP.
    $ NO.'I3'))
1001 FORMAT(T25'PROMOTE SEQUENCE POSITION'I3' TO'I3'
    $ (EQUIP. NO.'I3'))
1002 FORMAT(T25'EXCHANGE SEQUENCE POSITIONS'I3' AND'I3/T25
    1'(EQUIP. NO.'I3' AND NO.'I3'))
    END
```



```

C *****
C *
C *          SUBROUTINE DCHCK
C *
C * FUNCTIONS -
C *
C * - SEQUENCE CHANGE SEARCH ROUTINE
C * - ATTEMPTS TO FIND THE MOST BENEFICIAL CHANGE
C *   THAT CAN BE MADE TO THE CALCULATION SEQUENCE
C *   TO REDUCE RECYCLE ASSUMPTIONS
C * - PREVENTS ALTERNATING BETWEEN TWO SEQUENCES
C *
C *****

```

SUBROUTINE DCHCK (III, JJJ, IFLAG)

```

C***** THIS SUBROUTINE ATTEMPTS TO FIND THE MOST
C***** BENEFICIAL CHANGE THAT CAN BE MADE TO THE SEQUENCE
C***** TO REDUCE RECYCLE ASSUMPTIONS
C*****

```

```

      DIMENSION ISUM2(25)
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      COMMON /OPT1/IDELT(26,26), IREC(25), NOEQP, NP1, ISIGM
      IF (IDBUG(13)-4) 804, 800, 800
800 WRITE(IWRIT,1000) (IREC(I), I=1, NOEQP)
      WRITE(IWRIT,1001)
      DO 801 I=1, NP1
801 WRITE(IWRIT,1002) (IDELT(I, J), J=1, NP1)
804 CONTINUE

```

```

C***** STORE LAST MOVE (FOR PREVENTION OF SINGLE EXCHANGE
C***** CYCLING)

```

```

      IL=III
      JL=JJJ
      IFLAG=0

```

```

C***** IMAX- MAXIMUM POSSIBLE RECYCLE REDUCTION
C***** ENCOUNTERED SO FAR (EXCHANGE ONLY)

```

```

      IMAX=-1000

```

```

C***** INITIALIZE COLUMN SUMS (ISUM2(J)) TO ZERO
C***** COLUMN SUMS ARE UPDATED AS ROW SUMS ARE CALCULATED

```

```

      DO 1 J=1, NOEQP
1 ISUM2(J)=0

```

```

C***** HERE TO 2 STARTING AT BOTTOM OF 'IDELT', WORKING
C***** FROM DIAGONAL OUT, CALCULATE ROW SUMS, COL. SUMS,
C***** AND TOTAL SUMS & TEST FOR BEST MOVE

```


SUBROUTINE DCHCK ... (CONT'D)

```

DO 2 K=2,NOEQP
I=NOEQP-K+1
IP1=I+1
ISUM1=0
DO 2 J=IP1,NOEQP
ISUM1=ISUM1+IDELT(I,J)
ISUM2(J)=ISUM2(J)+IDELT(I,J)

```

```

C***** CHECK IF EXCHANGE WOULD RESULT IN GREATER RECYCLE
C***** REDUCTION THAN PREVIOUS MAXIMUM ENCOUNTERED (IMAX)

```

```

IF (ISUM1+ISUM2(J)-IDELT(I,J)-IMAX)3,4,4

```

```

C***** IF SAME EXCHANGE MADE LAST TIME - IGNORE

```

```

4 IF (1000*IL+JL-1000*I-J)5,3,5

```

```

C***** STORE MAX AND LOCATION

```

```

5 IMAX=ISUM1+ISUM2(J)-IDELT(I,J)
III=I
JJJ=J

```

```

C***** IF IMAX +VE, PROFITABLE EXCHANGE HAS BEEN FOUND -
C***** IGNORE PROMOTION/DEMOTION SEARCH

```

```

3 IF (IMAX)6,6,2

```

```

C***** IF ISUM1 +VE, PROFITABLE DEMOTION FOUND - FLAG
C***** AND STORE

```

```

6 IF (ISUM1)7,7,8
8 IFLAG=1
II=I
JJ=J

```

```

C***** IF ISUM2(J) +VE, PROFITABLE PROMOTION FOUND - FLAG
C***** AND STORE

```

```

7 IF (ISUM2(J))2,2,9
9 IFLAG=2
II=I
JJ=J
2 CONTINUE

```

```

C***** IFLAG=1 ADVANTAGE TO DEMOTING II TO JJ
C***** =2 ADVANTAGE TO PROMOTING JJ TO II
C***** =3 NULL OR NEGATIVE ADVANTAGE IN
C***** EXCHANGING III &
C***** JJJ (WILL BE USED IF NOTHING BETTER

```


SUBROUTINE DCHCK ... (CONT'D)

```
C*****      ENCOUNTERED)
C*****      =4      ADVANTAGE TO EXCHANGING III & JJJ
C*****      (HIGHEST PRIORITY IF IMAX +VE)

      IF(IMAX)20,20,21
20  IF(IFLAG) 22,22,23
23  III=II
      IJJ=JJ
      GO TO 999
22  IFLAG=3
      GO TO 999
21  IFLAG=4
999  CONTINUE
      RETURN
1000 FORMAT('O'T25'SIMPLIFIED SEQUENCE IS -'/(/T25,20I3))
1001 FORMAT('O'T25'IDELT MATRIX -'/)
1002 FORMAT(T25,20I3)
      END
```



```

C *****
C *
C *          SUBROUTINE FINSH
C *
C * FUNCTIONS -
C *
C * - OPTIMIZATION MONITOR ROUTINE
C * - DECIDES IF THE SEARCH FOR THE OPTIMUM
C *   SEQUENCE SHOULD BE CONTINUED UNINTERRUPTED,
C *   RENEWED WITH A RANDOMIZED SEQUENCE, OR
C *   TERMINATED
C * - STORES BEST SEQUENCE AS ENCOUNTERED
C * - RANDOMIZES THE CALCULATION SEQUENCE IF THIS IS
C *   REQUIRED -- REBUILDS ASSOCIATION MATRIX (VIA
C *   DELTA)
C *
C *****

```

SUBROUTINE FINSH (IFLAG,JFLAG)

```

C***** THIS SUBROUTINE DECIDES WHETHER THE SEARCH FOR THE
C***** OPTIMUM SEQUENCE SHOULD BE CONTINUED UNINTERRUPTED
C***** (JFLAG=1), RENEWED WITH A RANDOMIZED SEQUENCE
C***** (JFLAG=0), OR TERMINATED (JFLAG=2) IN THE ABSENCE
C***** OF DEBUG OPTIONS, IT ALSO CONTROLS PRINT-OUT OF
C***** BEST SEQUENCES AS ENCOUNTERED.
C*****

```

```

      DIMENSION JTEST(25)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /OPT1/IDELT(26,26),IREC(25),NOEQP,NP1,ISIGM
      DATA IX / 12345 /
      DATA IBEST,JCRIT/1000,5/

```

```

C***** INITIALIZE NULL IMPROVEMENT & RANDOMIZATION
C***** COUNTERS IF START OF SEARCH (IBEST=1000)

```

```

      IF(IBEST-1000) 51,50,51
50 LCOUN=0
   NCOUN=0

```

```

C***** IBEST IS THE BEST VALUE OF ISIGM ENCOUNTERED SO FAR
C***** IN THE SEARCH. IF A VALUE OF ISIGM BETTER (LOWER)
C***** IS RETURNED, SEQNC IS CALLED TO PRINT THE NEW BEST
C***** RESULTS AND IBEST IS REPLACED WITH ISIGM

```

```

      51 IF(ISIGM-IBEST) 100,101,101
      100 CALL SEQNC
         IBEST=ISIGM
      101 CONTINUE

```

```

C***** IF IFLAG IS NOT 3, AN ADVANTAGEOUS MOVE HAS BEEN

```


SUBROUTINE FINSH ... (CONT'D)

```

C***** FOUND AND SO JFLAG IS SET TO 1 TO CONTINUE WITH
C***** IMPROVEMENT VIA EXCHN
C***** IF IFLAG IS 3, A NULL OR NEGATIVE IMPROVEMENT IS
C***** THE BEST FOUND - A COUNTER LCOUN IS INCREMENTED.
C***** THIS COUNTER IS USED TO PREVENT CYCLING OF NULL
C***** MOVES (SAY A PERIOD OF 5 MOVES). WHEN THE COUNTER
C***** EXCEEDS A SPECIFIED VALUE, THE SEQUENCE IS
C***** RANDOMIZED AND THE SEARCH RENEWED FROM THE NEW
C***** STARTING POINT. THIS RANDOMIZATION PROCESS RESULTS
C***** IN ANOTHER COUNTER, NCOUN, BEING INCREMENTED. IF
C***** THIS COUNTER EXCEEDS A SPECIFIC VALUE, THE SEARCH
C***** IS TERMINATED

```

```

      IF(IFLAG-3) 10,11,10

```

```

C***** FLAG CONTINUE AND RETURN

```

```

10 JFLAG=1
   GO TO 999

```

```

C***** INCREMENT NULL IMPROVEMENT COUNTER

```

```

11 LCOUN=LCOUN+1
   IF(LCOUN-NOEQP) 10,12,12

```

```

C***** INCREMENT RANDOMIZATION COUNTER

```

```

12 NCOUN=NCOUN+1
   LCOUN=0
   IF(NCOUN-JCRIT) 13,14,14

```

```

C***** FLAG TERMINATION OF OPTIMIZATION AND RETURN

```

```

14 JFLAG=2
   GO TO 999

```

```

C***** FLAG RANDOMIZATION OF SEQUENCE

```

```

13 JFLAG=0

```

```

C***** HERE TO 42 RANDOMIZE THE SEQUENCE.

```

```

      DO 41 I=1,NOEQP
41 JTEST(I)=0
      DO 42 I=1,NOEQP
43 CALL RANDU(IX,IY,YFL)
      NO=YFL*NOEQP+0.5
      IX=IY
      IF(NO)43,43,45
45 IF(JTEST(NO)) 44,44,43

```


SUBROUTINE FINSH ... (CONT'D)

```
44 JTEST(NO)=1
   IREC(I)=IDELT(NP1,NO)
42 CONTINUE
   IF(IDBUG(13)-3) 801,800,800
800 WRITE(IWRIT,1001)
   WRITE(IWRIT,1000) (IREC(I),I=1,NDEQP)
801 CONTINUE

C***** CALL DELTA TO REBUILD THE 'IDELT' MATRIX FROM
C***** 'INFO' AND THE RANDOMIZED SEQUENCE

      CALL DELTA
999 CONTINUE
      RETURN
1000 FORMAT('O'T25'SIMPLIFIED SEQUENCE IS -'//'(T25,20I3))
1001 FORMAT('O'T25'SEQUENCE RANDOMIZED ')
      END
```



```

C *****
C *
C *          SUBROUTINE SEQNC
C *
C *  FUNCTIONS -
C *
C *  - REGENERATES A FULL CALCULATION SEQUENCE USING
C *    THE SIMPLIFIED SEQUENCE AND THE LINKS STORED
C *    BY REDUC
C *  - FINDS THE STREAMS WHICH MUST BE ASSUMED FOR THE
C *    COMPLETE CALCULATION SEQUENCE (FINAL CALCULATION
C *    SEQUENCE IF A BETTER SEQUENCE IS NOT ENCOUNTERED)
C *
C *****

```

SUBROUTINE SEQNC

```

C*****  THIS SUBROUTINE USES THE SIMPLIFIED SEQUENCE 'IREC'
C*****  AND THE MATRIX 'ILINK' TO BUILD THE TOTAL SEQUENCE
C*****  'ISEQ'. THIS SEQUENCE IS THEN PRINTED AND THE
C*****  STREAMS THAT MUST BE ASSUMED USING THAT CALCULATION
C*****  SEQUENCE ARE FOUND USING 'ISEQ' AND 'INFO', THEN
C*****  PRINTED
C*****  CALLED BY FINSH WHENEVER A BEST SEQUENCE 'IREC' IS
C*****  ENCOUNTERED (IE) NEW MINIMUM IBEST
C*****

```

```

COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /EXFC1/JTYPE(25),INDEX(25),ISEQ(25),IASUM(25)
$, ISUPR,IOPT
COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
COMMON /OPT1/IDELT(26,26),IREC(25),NOEQP,NP1,ISIGM
COMMON /OPT2/ILINK(25,2),LOCAL(25),KSUDO,KTOP,KBOT
IF(IOPT) 901,901,900

```

```

C*****  EQUATE NEQP ('ISEQ' LOCATION COUNTER) TO KTOP
C*****  (LOCATIONS 1 TO KTOP-1 HAVE BEEN FILLED PERMANENTLY
C*****  BY 'REDUC'

```

```

900 NEQP=KTOP

```

```

C*****  HERE TO 1 BUILD TOTAL SEQUENCE 'ISEQ' FROM
C*****  SIMPLIFIED SEQUENCE ('IREC')

```

```

DO 1 KSEQ=1,NOEQP

```

```

C*****  IEQP IS KSEQ ENTRY (LOCATION) IN IREC

```

```

IEQP=IREC(KSEQ)

```

```

C*****  IF IEQP=0, IGNORE (NEVER SHOULD OCCUR)

```


SUBROUTINE SEQNC ... (CONT'D)

IF(IEQP) 2,1,3

C***** IF IEQP IS +VE, ADD TO 'ISEQ' & INCREMENT NEQP

3 ISEQ(NEQP)=IEQP
NEQP=NEQP+1
GO TO 1

C***** IF IEQP -VE, FIRST CHANGE SIGN

2 IEQP=-IEQP

C***** HERE TO 4 LOOK FOR IEQP IN RHS OF ILINK MATRIX.

DO 4 I=1,25
IF(IEQP-ILINK(I,2)) 4,5,4

C***** IF ENCOUNTERED, LHS ENTRY MUST COME BEFORE IEQP IN
C***** ISEQ
C***** MAX OF ONE (PHASE 2-B) CAN OCCUR HERE FOR A GIVEN
C***** IREQ ENTRY

5 ISEQ(NEQP)=ILINK(I,1)
NEQP=NEQP+1
GO TO 6
4 CONTINUE

C***** ENTER IEQP IN 'ISEQ' & INCREMENT NEQP

6 ISEQ(NEQP)=IEQP
NEQP=NEQP+1

C***** JEQP - PARALLEL COUNTER - USED TO FIND END OF
C***** LINKED CHAIN

JEQP=NEQP

C***** HERE TO 7 LOOK FOR IEQP IN LHS OF 'ILINK' MATRIX

10 DO 7 I=1,25
IF(IEQP-ILINK(I,1)) 7,8,7

C***** IF ENCOUNTERED, ENTER RHS ENTRY INTO 'ISEQ' &
C***** INCREMENT NEQP (MAY BE MORE THAN ONE LHS 'ILINK'
C***** ENTRY = IEQP)

8 ISEQ(NEQP)=ILINK(I,2)
NEQP=NEQP+1
7 CONTINUE

SUBROUTINE SEQNC ... (CONT'D)

```

C***** IF NEQP & JEQP NOT EQUAL, MEANS ENTRY(S) FOUND IN
C***** 'ILINK'. THESE ENTRY(S) MUST BE CHECKED FOR FURTHER
C***** ENTRIES (IE) A CHAIN. IF ALL ENTRIES CHECKED,
C***** CONTINUE (LOOK AT NEXT 'IREC' ENTRY)

```

```
IF(NEQP-JEQP) 1,1,9
```

```

C***** EQUATE IEQP TO FIRST 'ISEQ' ENTRY NOT CHECKED & GO
C***** TO 10

```

```

9 IEQP=ISEQ(JEQP)
  JEQP=JEQP+1
  GO TO 10
1 CONTINUE

```

```
C***** CHECK FOR SEQUENCE BUILDING ERROR
```

```

IF(NEQP-1-KBOT) 12,11,12
12 WRITE(IWRIT,2000)
11 CONTINUE

```

```

C***** HERE TO 20 FIND STREAMS THAT MUST BE ASSUMED
C***** FOR PRESENT SEQUENCE - FOR EACH ENTRY IN 'ISEQ'
C***** FIND ALL INPUTS USING 'INFO' (ALL ORIGINAL NON-ZERO
C***** ,NON-PSEUDO-STREAMS) - IF SOURCE EQUIP OF INPUT
C***** DOES NOT OCCUR PREVIOUSLY IN 'ISEQ', STREAM MUST BE
C***** ASSUMED
C***** KASUM - ASSUMED STREAM COUNTER

```

```

901 KASUM=0
DO 30 I=1,25
30 IASUM(I)=0

```

```
C***** CHECK EACH ENTRY IN 'ISEQ'
```

```
DO 20 KREC=1,NNEQP
```

```

C***** CHECK NON-ZERO, NON-PSEUDO STREAMS IN 'INFO' FOR
C***** INTER-EQUIP INPUTS TO ISEQ(KREC)

```

```

DO 21 KSTRM=1,50
  IF(INFO(KSTRM,1)) 24,21,24
24 IF(INFO(KSTRM,3)-ISEQ(KREC)) 21,22,21

```

```

C***** CHECK IF INPUT SOURCE PREVIOUSLY ENCOUNTERED IN
C***** 'ISEQ'

```

```

22 DO 23 IEQP=1,KREC
  IF(INFO(KSTRM,2)) 27,21,27
27 IF(INFO(KSTRM,2)-ISEQ(IEQP)) 23,21,23

```


SUBROUTINE SEQNC ... (CONT'D)

23 CONTINUE

C***** STORE ASSUMED STREAM

KASUM=KASUM+1

IASUM(KASUM)=KSTRM

21 CONTINUE

20 CONTINUE

IF(IOPT) 950,950,879

879 IF(IDBUG(13)-1) 881,880,880

880 WRITE(IWRIT,2001) (ISEQ(I),I=1,NNEQP)

IF(KASUM) 25,25,26

C***** PRINT STREAMS WHICH MUST BE ASSUMED USING THIS

C***** SEQUENCE, IF ANY

26 WRITE(IWRIT,2002) (IASUM(I),I=1,KASUM)

25 CONTINUE

881 CONTINUE

RETURN

950 WRITE(IWRIT,4000) (ISEQ(I),I=1,NNEQP)

IF(KASUM) 952,952,953

953 WRITE(IWRIT,2002) (IASUM(I),I=1,KASUM)

GO TO 951

952 WRITE(IWRIT,4002)

951 WRITE(IWRIT,9000)

RETURN

2000 FORMAT(1H,'ERROR IN SEQUENCE BUILDING')

2001 FORMAT('0'T40'FOR THE CALCULATION SEQUENCE -'/(/T25
\$,20I3))2002 FORMAT('0'T35'THE FOLLOWING STREAMS MUST BE ASSUMED,'
\$/(/T40,10I3))4000 FORMAT('1'////T37'THE GIVEN CALCULATION SEQUENCE IS -'
\$/
1(/T25,20I3))

4002 FORMAT('0'T42'NO STREAMS NEED BE ASSUMED.'/)

9000 FORMAT('0',T25,'*****
\$*****

1*****' /)

END


```

C *****
C *
C *          SUBROUTINE RXWHB
C *
C * FUNCTIONS -
C *
C * - PRIMARY REACTION FURNACE--WASTE HEAT BOILER
C * ROUTINE
C * - INITIALIZES CALCULATIONS -- DESIGNS OR SIMULATES
C * THE COMBUSTION CHAMBER, AND ONE, TWO OR THREE
C * BOILER PASSES
C * - CALCULATES ONE, TWO OR THREE BYPASS STREAMS IF
C * THEY EXIST AND STORES THE MAIN BOILER EXIT STREAM
C * - FINDS STEAM PRODUCTION AND SULPHUR CONVERSION
C *
C *****

```

```

SUBROUTINE RXWHB
DIMENSION NBYP(3)
COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
COMMON /GEN2/TEMP, TFEED, YCOMP(20), YFEED(20), PRESS, ENTH
COMMON /DATA5/IDH2O, IDSUL(5), WTMOL(20), VMOL(20)
COMMON /STOR1/EQUIP(300), ILOC, NMREQ, STREM(50,22)
$, NSIN(5), NSOUT(5)
COMMON /HTLS1/TNUMB, TDIAM, TLONG, TSHL1, TSHL2, QLOSS
$, DELPC, DELTP
COMMON /BURN2/IFLAG, IPASS, MPASS, ESTMT(3)
WRITE(IWRIT,6000) NMREQ

```

```

C***** CALL BINIT TO INITIALIZE BOILER CALCULATIONS

```

```

CALL BINIT(NSTMS, NSTMP, PSTEM, NBYP, NEXIT, NOPAS)

```

```

C***** CALL BRXNC TO DESIGN / SIMULATE RXN. CHAMBER.

```

```

CALL BRXNC
IF(ITEST-1) 811, 810, 810
810 WRITE(IWRIT,9001)
811 CONTINUE
IPASS=1
MPASS=0

```

```

C***** DEFINE IFLAG FOR PASS

```

```

1 CALL FLAGI(IPASS+MPASS)

```

```

C***** DEFINE JFLAG FOR PASS.

```

```

CALL FLAGJ(JFLAG, NBYP, NOPAS)
CALL DOPAS (JFLAG, NOPAS)

```

```

C***** CHECK FOR BYPASS STREAM(S).

```


SUBROUTINE RXWHB ... (CONT'D)

```

      IF(NOPAS-IPASS) 47,28,1
28  NCNT=3
29  IF(NBYP5(NCNT)) 30,30,31
30  NCNT=NCNT-1
      IF(NCNT) 1,1,29
31  NPLAC=ILOC+(17+NCNT*2)
      BYPAS=SETVU(ABS(EQUIP(NPLAC)),0.1)
      DO 49 I=1,NGMS
        YFEED(I)=YCOMP(I)*(1.0-BYPAS)
49  YCOMP(I)=YCOMP(I)*BYPAS
      CALL SUTIL (NBYP5(NCNT),2,YCOMP,TEMP,PRESS)
      DO 60 I=1,NGMS
60  YCOMP(I)=YFEED(I)
      IF(ITEST-1) 801,800,800
800  WRITE(IWRIT,5000) NCNT,BYPAS
      CALL PRNT5(NBYP5(NCNT))
      IF(NCNT-1) 805,805,801
805  WRITE(IWRIT,5001)
801  CONTINUE
      IF(NCNT-1) 1,1,30
47  IF(IPASS-NOPAS) 1,1,50
50  CONTINUE

```

C***** DEFINE STREAM EXIT BOILER.

```

      CALL SUTIL (NEXIT,2,YCOMP,TEMP,PRESS)
      TDEWS=500.
      CALL DEWPT(TDEWS,YCOMP,PRESS,1)
      TDEWW=150.
      CALL DEWPT(TDEWW,YCOMP,PRESS,0)
      IF(ITEST-1) 803,802,802
802  WRITE(IWRIT,5050)
      CALL PRNT5(NEXIT)
      WRITE(IWRIT,5002) TDEWS,TDEWW
      WRITE(IWRIT,9000)
803  CONTINUE

```

C***** CALCULATE BOILER STEAM PRODUCTION RATE.

```

      DUTY=EQUIP(ILOC+28)
      CALL STEAM(DUTY,TSHL1,PSTEM,NSTMS,NSTMP,27)
      DO 100 J=1,3
        NSTRM=NBYP5(J)
        IF(NSTRM) 100,100,101
101  CALL SUTIL(NSTRM,1,YFEED,TFEED,PFEED)
        DO 102 I=1,NTOT
102  YCOMP(I)=YCOMP(I)+YFEED(I)
100  CONTINUE
      CALL PRNT(2)
      RETURN

```


SUBROUTINE RXWHB ... (CONT'D)

```
5000 FORMAT(///,T33,'BOILER BY-PASS NO.'I3' , (RATIO = '
      $,F7.4,'))
5001 FORMAT('1')
5002 FORMAT(//T35'STREAM SULPHUR DEW PT. (DEG. F) = ',F7.1
      $/T35'STREAM W
      LATER DEW PT. (DEG. F) = ',F7.1)
5050 FORMAT(///T45,'BOILER EXIT STREAM -')
6000 FORMAT(T34,'COMBUSTION REACTION AND WASTE HEAT
      $ BOILER.'/T45
      1,'EQUIPMENT NUMBER 'I3)
9000 FORMAT('0',T25,'*****
      $*****
      1*****'/ )
9001 FORMAT('1')
      END
```



```

C *****
C *
C *          SUBROUTINE BINIT
C *
C *  FUNCTIONS -
C *
C *  -  BOILER INITIALIZATION ROUTINE
C *  -  INITIALIZES BOILER CALCULATIONS -- DEFINES
C *      BOILER FEED, EQUILIBRIUM CUTOFF TEMPERATURE,
C *      BYPASS AND EXIT STREAMS, STEAM STREAMS AND
C *      BOILER STEAM PRESSURE
C *  -  CALCULATES BOILER STEAM TEMPERATURE, CHECKS
C *      DATA COMPATIBLTY AND FLAGS WHETHER A MUFFLE
C *      FURNACE OR A FIRE TUNNEL IS USED
C *
C *****

```

```

SUBROUTINE BINIT(NSTMS,NSTMP,PSTEM,NBYP,NEXIT,NOPAS)
DIMENSION YSTEM(20),NBYP(3)
COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)
COMMON /STOR1/EQUIP(300),ILOD,NMBEQ,STREM(50,22)
$,NSIN(5),NSOUT(5)
COMMON /HTLS1/TNUMB,TDIAM,TLONG,TSHL1,TSHL2,QLOSS
$,DELPC,DELTP
COMMON /BURN1/TCTOF,TBURN,IMUFF,NLGTH,NDIAM,NRTIM
$,NHRLS,NBURN
COMMON /BURN2/IFLAG,IPASS,MPASS,ESTMT(3)
COMMON /FLOW1/INFO(75,5),NNEQP,NOSTM
NOPAS=ABS(EQUIP(ILOD+1))+0.5
ESTMT(1)=1400.
ESTMT(2)= 900.
ESTMT(3)= 600.

```

```

C*****      TCTOF SPECIFIED OR ELSE 1100. DEG. F.

```

```

TCTOF=SETVU(-EQUIP(ILOD+25),1100.0)
EQUIP(ILOD+25)=SIGN(TCTOF,EQUIP(ILOD+25))

```

```

C*****      DEFINE COMBUSTION FEED.

```

```

NSTRM=0
CALL SUTIL (NSTRM,0,YFEED,TFEED,PRESS)
CALL PRNT(1)
CALL PRNTS(-1)

```

```

C*****      DEFINE BYPASS STREAM(S) IF PRESENT.

```

```

NCNT=0
DO 21 I=1,3
NPLAC=ILOD+(18+I*2)

```


SUBROUTINE BINIT ... (CONT'D)

```

    NBYPS(I)=-EQUIP(NPLAC)
    IF(NBYPS(I)) 21,21,20
20  NCNT=NCNT+1
21  CONTINUE

```

C***** DEFINE STEAM SOURCE STREAM IF PRESENT.

```

    NSTMS=0
    IF(INFO(NSTRM,5)) 23,23,22
22  NSTMS=NSTRM
23  CONTINUE

```

C***** DEFINE PRIMARY EXIT STREAM.

```

    DO 24 I=1,4
    NEXIT=NSOUT(I)
    DO 25 J=1,NCNT
    IF(NEXIT-NBYPS(J)) 25,24,25
25  CONTINUE
    GO TO 26
24  CONTINUE

```

C***** DEFINE STEAM PRODUCT STREAM IF PRESENT.

```

26  NSTMP=IABS(NSOUT(NCNT+2))

```

C***** COMPARE BOILER OUTLET TEMP., BYPAS TEMP. AND STEAM
C***** PRESS. DATA FOR COMPATIBILITY.

```

    DO 17 I=1,NCNT
17  CALL COMPR(NBYPS(I),21,7+NOPAS)
    CALL COMPR(NEXIT,21,8+NOPAS)
    CALL COMPR(NSTMP,22,27)
    CALL COMPR(NSTMS,22,27)

```

C***** DEFINE BOILER STEAM STREAM

```

    CALL SUTIL (NSTMP,1,YSTEM,TSTEM,PSTEM)

```

C***** STEAM TEMP. ESTIMATED OR GUESSED 450.0 DEG. F.

```

    TSTEM=SETVU(TSTEM,450.0)

```

C***** STEAM PRESSURE SPECIFIED OR 250.0 PSIA.

```

    PSTEM=SETVU(-EQUIP(ILOC+27),250.0)

```

C***** MAKE SURE SOME H2O IS IN STREAM .

```

    YSTEM(IDH2O)=SETVU(YSTEM(IDH2O),1.0)

```


SUBROUTINE BINIT ... (CONT'D)

C***** CALCULATE SATURATED STEAM TEMP.

CALL DEWPT(TSTEM,YSTEM,PSTEM,0)

TSHL1=TSTEM

TSHL2=TSTEM

C***** CHECK IF MUFFLE FURNACE EXISTS & FLAG.

C***** IF ONE EXISTS, TLONG MUST BE SPECIFIED.

C***** IF ONE DOES NOT EXIST, FIRST PASS TNUMB=1.

IMUFF=0

NBURN=ILOC+26

NLGTH=ILOC+2

NDIAM=ILOC+6

IF(EQUIP(ILOC+2)) 12,11,11

12 IF(ABS(EQUIP(ILOC+3)+1.0)-1.0E-2) 11,11,13

13 IMUFF=1

NLGTH=ILOC+17

NDIAM=ILOC+18

11 CONTINUE

NRTIM=ILOC+15

NHRLS=ILOC+16

NDUTY=ILOC+28

EQUIP(NDUTY)=0.0

RETURN

END


```

C *****
C *
C *          SUBROUTINE DOPAS
C *
C * FUNCTIONS -
C *
C * - BOILER TUBE PASS CALCULATION ROUTINE
C * - SIMULATES OR DESIGNS BOILER TUBE PASSES
C * - SIMULATION -- SINGLE PASS NON-ADIABATIC
C *   TEMPERATURE CALCULATION
C * - DESIGN -- SINGLE OR MULTIPLE PASSES -- ITERATIVE
C *   TUBE NUMBER DETERMINATION
C * - CALCULATES PRESSURE DROP AND/OR TUBE DIAMETER
C *   FOR EACH PASS
C * - CALCULATES BOILER HEAT LOAD (DUTY)
C *
C *****

```

```

      SUBROUTINE DOPAS (JFLAG,NOPAS)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /HTLS1/TNUMB,TDIAM,TLONG,TSHL1,TSHL2,GLOSS
      $,DELPC,DELTP
      COMMON /BURN2/IFLAG,IPASS,MPASS,ESTMT(3)
2    CONTINUE
      NOHLS=1
      IF(JFLAG-1) 3,3,4
      4 IF(ITEST-2) 801,800,800
800  IF(MPASS) 305,305,306
305  WRITE(IWRIT,3005) IPASS
      GO TO 801
306  WRITE(IWRIT,3006)
801  CALL NCALC
      IFLAG=1
      JFLAG=1
      TEMP=ESTMT(IPASS)
      GO TO 2
      3 IF(ITEST-2) 803,802,802
802  WRITE(IWRIT,3010) IPASS
803  CALL TCALC(NOHLS)
      IF(ITEST-1) 805,804,804
804  IF(NOPAS-IPASS) 10,10,11
      11 CALL PRNTS(0)
      GO TO 12
      10 WRITE(IWRIT,9000)
      12 WRITE(IWRIT,9001)
805  CONTINUE
      NUMBT=ILOC+IPASS+8
      NUMBN=ILOC+IPASS+2
      NUMBP=ILOC+IPASS+11

```


SUBROUTINE DOPAS ... (CONT'D)

```

NUMBD=ILOC+IPASS+5
EQUIP(NUMBT)=SIGN(TEMP,EQUIP(NUMBT))
EQUIP(NUMBN)=SIGN(TNUMB,EQUIP(NUMBN))
EQUIP(NUMBD)=-TDIAM
EQUIP(NUMBP)=DELPC
DO 30 I=1,NGMS
30 YFEED(I)=YCOMP(I)
   TFEED=TEMP
   NDUTY=ILOC+28
   EQUIP(NDUTY)=EQUIP(NDUTY)+QLOSS
   IF(MPASS) 46,46,45
45 MPASS=MPASS-1
   IPASS=IPASS+1
   JFLAG=2
   NUMBT=ILOC+IPASS+MPASS+8
   TEMP=-EQUIP(NUMBT)
   CALL FLAGI(IPASS)
   GO TO 2
46 CONTINUE
   IPASS=IPASS+1
   RETURN
3005 FORMAT(///T44,'DESIGN OF PASS NO. ',I2)
3006 FORMAT(///T42,'MULTIPLE TUBE PASS DESIGN.')
```

3010 FORMAT(///T40,'SIMULATION OF TUBE PASS NO. ',I2)

```

9000 FORMAT('D',T25,'*****')
      $*****
      1*****')/
9001 FORMAT('1')
      END
```



```

C *****
C *
C *          SUBROUTINE FLAGI
C *
C *  FUNCTIONS -
C *
C *  -  IFLAG UTILITY ROUTINE
C *  -  SETS THE FLAG IFLAG FOR THE PASS (1 FOR
C *      DIAMETER SPECIFIED, PRESSURE DROP TO BE
C *      CALCULATED, 2 FOR TUBE DIAMETER AND PRESSURE
C *      DROP TO BE CALCULATED)
C *  -  SETS BOILER LENGTH
C *
C *****

```

```

SUBROUTINE FLAGI(ICNT)
COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
COMMON /STOR1/EQUIP(300), ILOC, NMREQ, STREM(50,22)
$, NSIN(5), NSOUT(5)
COMMON /HTLS1/TNUMB, TDIAM, TLONG, TSHL1, TSHL2, QLOSS
$, DELPC, DELTP
COMMON /BURN1/TCTOF, TBURN, IMUFF, NLGTH, NDIAM, NRTIM
$, NHRLS, NBURN
COMMON /BURN2/IFLAG, IPASS, MPASS, FSTMT(3)
TLONG=SETVU(ABS(EQUIP(ILOC+2)),20.)
NUMBD=ILOC+ICNT+5
NUMBP=ILOC+ICNT+11

```

```

C*****  ALWAYS SIMULATE FIRST PASS IF NO MUFFLE FURNACE
C*****  PRESENT.

```

```

      IF(IPASS+IMUFF-1) 1,1,11
1  TDIAM=ABS(EQUIP(ILOC+6))
   IFLAG=1
   RETURN

```

```

C*****  IF TDIAM SPECIFIED, CALCULATE DELPC.

```

```

      11 IF(EQUIP(NUMBD)) 2,3,3

```

```

C*****  SIMULATION CASE.

```

```

      2 IFLAG=1
      TDIAM=-EQUIP(NUMBD)

```

```

C*****  IF DELTP ALSO SPECIFIED - ERROR.
C*****  (ASSUME DESIGN CASE IN THIS EVENT).

```

```

      IF(EQUIP(NUMBP)) 4,5,5
      5 RETURN

```

```

C*****  IF DELTP SPECIFIED, CALCULATE TDIAM

```


SUBROUTINE FLAGI ... (CONT'D)

```
C***** IF NEITHER SPECIFIED, - ASSUME DELTP (DESIGN
C***** CASE).
```

```
3 IF(EQUIP(NUMBP)) 6,10,10
```

```
C***** DESIGN CASE.
```

```
6 IFLAG=2
  DELTP=-EQUIP(NUMBP)
  RETURN
```

```
C***** IF NEITHER SPEC. GIVEN, ASSUME DESIGN CASE.
C***** (SPECIFY DELTP= 0.40 PSIA.)
```

```
10 IFLAG=2
  DELTP=0.4
  RETURN
```

```
C***** IF BOTH SPECS. GIVEN, ASSUME DESIGN CASE.
```

```
4 WRITE(IWRIT,5000)
  IFLAG=2
  DELTP=-EQUIP(NUMBP)
  RETURN
```

```
5000 FORMAT('0 INVALID BOILER SPECS. -'/ ' ONE AND ONLY
$ ONE OF TDIAM 0
1R DELTP MUST BE SPECIFIED FOR EACH BOILER TUBE PASS.')
END
```



```

C *****
C *
C *          SUBROUTINE FLAGJ
C *
C *  FUNCTIONS -
C *
C *  -  JFLAG UTILITY ROUTINE
C *  -  SETS THE FLAG JFLAG FOR THE TUBE PASS (1 FOR
C *      SIMULATION -- (TUBE NUMBER GIVEN, EXIT
C *      TEMPERATURE TO BE CALCULATED), 2 FOR DESIGN --
C *      (EXIT TEMPERATURE GIVEN, TUBE NUMBER TO BE
C *      DETERMINED)
C *  -  DEFINES ESTIMATE FOR EITHER EXIT TEMPERATURE
C *      OR TUBE NUMBER
C *  -  FLAGS FOR MULTIPLE TUBE PASS DESIGN IF THIS IS
C *      TO BE DONE
C *
C *****

```

```

      SUBROUTINE FLAGJ(JFLAG,NBYP,NOPAS)
      DIMENSION NBYP(3)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /HTLS1/TNUMB,TDIAM,TLONG,TSHL1,TSHL2,QLOSS
      $,DELPC,DELTP
      COMMON /BURN1/TCTOF,TBURN,IMUFF,NLGTH,NDIAM,NRTIM
      $,NHRLS,NBURN
      COMMON /BURN2/IFLAG,IPASS,MPASS,ESTMT(3)
1  ICNT=IPASS+MPASS
      NUMBT=ILOC+ICNT+3
      NUMBN=ILOC+ICNT+2

```

```

C*****      ALWAYS SIMULATE FIRST PASS IF NO MUFFLE FURNACE
C*****      PRESENT.

```

```

      IF(IPASS+IMUFF-1) 2,2,3
2  TEMP=1700.
      TNUMB=1
      JFLAG=1
      RETURN

```

```

C*****      IF TNUMB SPECIFIED, CALCULATE TEMP.

```

```

      3 IF(EQUIP(NUMBN)) 8,9,9

```

```

C*****      SIMULATION CASE.

```

```

      8 JFLAG=1
      TNUMB=-EQUIP(NUMBN)

```


SUBROUTINE FLAGJ ... (CONT'D)

```

C***** IF TEMP ALSO SPECIFIED, - ERROR.
C***** IF TEMP ESTIMATE GIVEN, USE IT.
C***** OTHERWISE GENERATE TEMP GUESS.

      IF(EQUIP(NUMBT)) 50,11,12
11 TEMP=ESTMT(ICNT)
   GO TO 13
12 TEMP=EQUIP(NUMBT)

C***** CHECK FOR MULTIPLE PASS SIMULATION ATTEMPT.
C***** (MULTIPLE PASS CALCULATIONS DONE ONLY FOR DESIGN)

13 IF(MPASS) 14,14,51
14 RETURN

C***** IF TEMP SPECIFIED, CALCULATE TNUMB
C***** IF NEITHER SPEC GIVEN, ASSUME MULTIPLE PASS DESIGN

      9 IF(EQUIP(NUMBT)) 20,30,30
20 JFLAG=2
   TEMP=-EQUIP(NUMBT)

C***** IF TUBE ESTIMATE GIVEN, USE IT
C***** (OTHERWISE GENERATE A TUBE NUMBER GUESS)

25 IF(EQUIP(NUMBN)) 22,22,23
22 TNUMB=50.
   GO TO 24
23 TNUMB=EQUIP(NUMBN)
24 RETURN

C***** SIMULTANEOUS MULTIPLE TUBE PASS DESIGN CASE.

30 MPASS=MPASS+1

C***** CHECK FOR LAST TUBE PASS - ERROR.

      IF(IPASS+MPASS-NOPAS) 31,31,32
32 WRITE(IWRIT,5002)

C***** ASSUME FINAL TUBE PASS OUTLET TEMP.

40 TEMP=ESTMT(ICNT)
   JFLAG=2
   MPASS=MPASS-1
   GO TO 25

C***** CHECK THAT BYPASS NOT INCLUDED IN MULTIPLE DESIGN.
C***** (IF BYPASS DESIRED, BYPASS TEMP. MUST BE SPEC.).

```


SUBROUTINE FLAGJ ... (CONT'D)

```

31 DO 34 I=1,3
   IF(NBYP5(I)) 34,34,33
34 CONTINUE
   GO TO 1
33 IF(IPASS+MPASS-NOPAS+1) 1,1,35
35 WRITE(IWRIT,5003)
   GO TO 40

```

```

C*****      IF BOTH TNUMB AND TEMP SPECIFIED, ASSUME DESIGN
C*****      CASE.

```

```

50 WRITE(IWRIT,5004)
   GO TO 52

```

```

C*****      IF MULTIPLE PASS SIMULATION ATTEMPT, ASSUME DESIGN
C*****      CASE.

```

```

51 WRITE(IWRIT,5005)
52 JFLAG=2
   TEMP=ESTMT(ICNT)
   GO TO 25
5003 FORMAT('O  INVALID BOILER SPECS.  -'/'  BYPAS STREAM
$ MAY NOT BE
1 INCLUDED IN MULTIPLE TUBE PASS DESIGN.'/'  (BYPASS
$ STREAM TEMP.
1 MUST BE SPECIFIED.))
5002 FORMAT('O  INVALID BOILER SPECS.  -'/'  FOR DESIGN
$ CASE AT LEAST
1 THE LAST OUTLET TEMP. MUST BE SPECIFIED.))
5005 FORMAT('O  INVALID BOILER SPECS.  -'/'  MULTIPLE PASS
$ SIMULATION
1 CANNOT BE DONE ,  GIVE EACH TNUMB FOR SIMULATION.))
5004 FORMAT('O  INVALID BOILER SPECS.  -'/'  AT MOST ONLY
$ ONE OF TEMP
1 OR TNUMB MAY BE SPECIFIED FOR A GIVEN PASS.))
END

```



```

C *****
C *
C *          SUBROUTINE NCALC
C *
C *  FUNCTIONS -
C *
C *  -  BOILER TUBE NUMBER DETERMINATION ROUTINE
C *  -  CALCULATES COMPOSITION AT SPECIFIED TUBE
C *      PASS EXIT TEMPERATURE
C *  -  CALCULATES HEAT LOSS FOR EACH ESTIMATED TUBE
C *      NUMBER -- ITERATES ON TUBE NUMBER UNTIL DESIRED
C *      HEAT LOSS IS ACHIEVED
C *  -  FOR EACH ESTIMATE TUBE DIAMETER AND/OR
C *      PRESSURE DROP ARE CALCULATED
C *  -  FOR MULTIPLE TUBE PASS DESIGN, CALCULATES
C *      TOTAL HEAT LOSS FOR TUBE PASSES INVOLVED, USING
C *      AVERAGED COMPOSITION AND ESTIMATED INTERMEDIATE
C *      TUBE PASS EXIT TEMPERATURES -- TUBE PASSES
C *      INVOLVED ARE ASSUMED IDENTICAL
C *
C *****

```

```

SUBROUTINE NCALC
  DIMENSION YAVG(20)
  COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
  COMMON /GEN2/TEMP, TFEED, YCOMP(20), YFEED(20), PRESS, ENTH
  COMMON /HTLS1/TNUMB, TDIAM, TLONG, TSHL1, TSHL2, GLOSS
  $, DELPC, DELTP
  COMMON /BURN2/IFLAG, IPASS, MPASS, ESTMT(3)
  DATA TWALL/500./
  TINTR(I1,I2)=((TFEED-TSHL1)**I1*(TEMP-TSHL2)**I2)**(1.
  $/(I1+I2))+
  1 (TSHL1+TSHL2)/2.

```

```

C*****  CALCULATE REFERENCE ENTHALPY OF INLET STREAM AT
C*****  INLET TEMP.

```

```

  ENTHR=HFCAL(TFEED,YFEED,0)

```

```

C*****  CALCULATE COMPOSITION AT SPECIFIED OUTLET TEMP.,
C*****  (TEMP).

```

```

  KINIT=1
  LOOSE=1
  CALL COMP(LOOSE,KINIT)

```

```

C*****  CALCULATE STREAM ENTHALPY AT SPECIFIED OUTLET
C*****  TEMP.

```

```

  ENTH=HFCAL(TEMP,YCOMP,0)
  IF(ITEST-3) 811,810,810
810 WRITE(IWRIT,5010) TFEED,ENTHR

```


SUBROUTINE NCALC ... (CONT'D)

```
WRITE(IWRIT,5000) TEMP,ENTH
811 CONTINUE
```

```
C***** EVALUATE STREAM PROPERTIES NEEDED FOR QLOSS CALC.
```

```
CALL PROP(TWALL,YAVG,AVGMU,WALMU,RHO,TMASS,YTOT,CPAVG)
```

```
C***** SET UP INTERMEDIATE TEMPERATURES IF NECESSARY
C***** * (MULTIPLE TUBE PASS DESIGN).
```

```
NTIME=MPASS+1
NFINL=IPASS+MPASS
ESTMT(NFINL)=TEMP
TFSTR=TFEED
IF(MPASS-1) 23,21,22
21 ESTMT(IPASS)=TINTR(1,1)
GO TO 23
22 ESTMT(IPASS)=TINTR(2,1)
ESTMT(IPASS+1)=TINTR(1,2)
23 CONTINUE
FAC1=1.5
FAC2=0.5
ITERH=0
```

```
C***** GENERATE A GUESS FOR THE NUMBER OF TUBES.
```

```
1 CALL GUESR(TNUMB,FAC1,FAC2,ERROR,ITERH)
```

```
C***** CALCULATE RESULTING ERROR.
C***** CALCULATE PRESSURE DROP. (FOR SIMULATION, ALSO SET
C***** DIAMETER.)
```

```
CALL PDROP(AVGMU,WALMU,RHO,TMASS,GT,ITERH)
DELPC=DELPC*NTIME
QLOSS=0.
DO 20 IIIII=1,NTIME
JJJJJ=IIIII+IPASS-1
TEMP=ESTMT(JJJJJ)
```

```
C***** CALCULATE TOTAL HEAT LOSS FOR PASS.
```

```
CALL HLOSS (GT,CPAVG,TWALL,YTOT,YAVG)
TFEED=TEMP
20 CONTINUE
TFEED=TFSTR
```

```
C***** DEFINE ERROR AS REFERENCE ENTHALPY MINUS (ENTHALPY
C***** AT THE GUESSED TEMP + HEAT LOSS).
```

```
ERROR=ENTHR-ENTH-QLOSS
```


SUBROUTINE NCALC ... (CONT'D)

```

      IF(ITEST-3) 817,816,816
816  WRITE(IWRIT,5011) TNUMB,QLOSS,ERROR
817  CONTINUE

```

```

C*****  CONVERGENCE CHECK.

```

```

      IF(ABS(ERROR/ENTH)-CRIT) 2,2,1

```

```

C*****  ROUND NUMBER OF TUBES TO AN INTEGER NUMBER.

```

```

      2  NTUBE=TNUMB+0.5
        TNUMB=NTUBE
        IF(ITEST-2) 801,800,800
800  WRITE(IWRIT,3007)
        IF(IFLAG-1) 303,303,304
303  WRITE(IWRIT,3002)
        GO TO 310
304  WRITE(IWRIT,3003)
310  WRITE(INPIT,9000)
        WRITE(IWRIT,4002) TNUMB,TDIAM,TLONG
        WRITE(IWRIT,4003) DELPC,QLOSS,ERROR
        WRITE(IWRIT,9000)
801  CONTINUE
        RETURN
3002  FORMAT(T37,'TDIAM SPECIFIED,      DELPC CALCULATED.')
```

```

3003  FORMAT(T37,'DELTP SPECIFIED,      TDIAM CALCULATED.')
```

```

3007  FORMAT(    /T32,'ITERATIVE CALCULATION OF TUBE-PASS
$ TUBE-NUMBER')
```

```

4002  FORMAT(  T40,'CONVERGED TUBE NUMBER IS ',F5.0/T41'TUBE
$ DIAMETER (I
1N) IS ',F6.2/T42'TUBE LENGTH (FT) IS ',F6.2/)
```

```

4003  FORMAT(T38,'APPROX. PRESS. DROP (PSI.) = ',F6.2
$/T31'APPROX. TOTAL
1HEAT LOSS (BTU.) = ',E15.7/T36,'(ENTH. ERROR (BTU.) =
$ ',E15.7' )'/
1/T34,'REVERT TO SIMULATION FOR EXACT CALCULATION'
$/T36'OF ACTUAL DU
1TLET TEMP. AND PRESS. DROP')
```

```

9000  FORMAT('0',T25,'*****')
1'*****'/ )
```

```

5000  FORMAT(1H0,'SPEC TEMP. = ',F10.4,' DEG. F,
$ OBJECTIVE ENTHALPY
1IS ',E15.7,' BTU.'/)
```

```

5010  FORMAT(1H0,'FEED TEMP. = ',F10.4,' DEG. F,
$ REFERENCE ENTHALPY
1IS ',E15.7,' BTU.'/)
```

```

5011  FORMAT(1H0,'*****  TNUMB = ',F10.4,' , QLOSS = '
$,E15.7/T28,' F
1RROR = ',E15.7)
      END

```



```

C *****
C *
C *          SUBROUTINE HLOSS
C *
C *  FUNCTIONS -
C *
C *  -  BOILER TUBE PASS HEAT LOSS CALCULATION ROUTINE
C *  -  CALCULATES TOTAL HEAT LOSS (CONVECTIVE AND
C *      RADIATIVE) FOR A SINGLE PASS
C *  -  IGNORES RADIATION EFFECT IF AVERAGE STREAM
C *      TEMPERATURE IS LESS THAN 900 DEG. F
C *  -  USES GIVEN FEED TEMPERATURE, AVERAGE TUBE PASS
C *      COMPOSITION AND EITHER SPECIFIED OR ESTIMATED
C *      TUBE EXIT TEMPERATURE FOR CALCULATION OF HEAT
C *      LOSS
C *  -  CALCULATES EMISSIVITY AND ABSORPTIVITY OF GAS
C *      BY LINEAR INTERPOLATION
C *
C *****

```

```

      SUBROUTINE HLOSS (GT,CPAVG,TWALL,YTOT,YAVG)
      DIMENSION YAVG(20),EPS(4),RPL(4)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /DATA4/RMU(20),SMU(20),RADCT(20)
      COMMON /HTLS1/TNUMB,TDIAM,TLONG,TSHL1,TSHL2,QLOSS
      $,DELPC,DELTP
      DATA RPL,EPS /-3.912023005,-2.525728644,
      $-1.609437912
      1,1.386294361,4.219507705,5.075173815,5.480638923
      $,6.802394763/
      IF(ITEST-5) 811,810,810
      810 WRITE(IWRIT,9999)
      9999 FORMAT(1H0,' TOTAL TUBE PASS HEAT LOSS CALC 'HLOSS')
      $          '/')
      811 CONTINUE

```

```

C*****  CALC. CONVECTIVE HEAT TRANSFER COEFFICIENT, UCONV
C*****  AND CONVECTIVE HEAT LOSS, QCONV
C*****  ASSUME STEAM FILM COEFF., GAS SIDE FOULING RESIST.
C*****  , STEAM SIDE FOULING RESIST., AND METAL WALL
C*****  THERMAL RESIST.
C*****  REF. - VALDES

```

```

      HS=2000.
      RGF=0.005
      RM=0.0001
      RS=0.0005
      HG=16.6*(GT/3600.)**0.8*CPAVG/TDIAM**0.2
      UCONV = 1 / (1/HG + RGF + RM + RS + 1/HS)
      AREA=3.14159*TDIAM/12.0*TLONG*TNUMB
      DTLM=((TFEED-TSHL1)-(TEMP -TSHL2))

```


SUBROUTINE HLOSS ...(CONT'D)

```
1 /ALOG((TFEED-TSHL1)/(TEMP -TSHL2))
```

```
QCONV=UCONV*AREA*DTLM
```

```
C***** IGNORE RADIATION LOSSES IF TEMP LESS THAN 900.  
C***** DEG. F.
```

```
QRAD=0.0
```

```
TMEAN=(TFEED+TEMP)/2.0
```

```
IF(TMEAN-900.) 20,10,10
```

```
C***** CALCULATE RADIATION HEAT LOSS  
C***** ASSUME PIPE WALL EMISSIVITY IS 0.8  
C***** ASSUME RADIATING GAS TEMP IS MEAN OF TUBE END  
C***** TEMPERATURES.
```

```
10 CONTINUE
```

```
EPSP=0.8
```

```
C***** CALCULATE EMISSIVITY OF RADIATING COMPONENTS AT  
C***** MEAN STREAM TEMP. AND ABSORPTIVITY OF GAS AT WALL  
C***** TEMP. (SULPHUR DEW PT.)  
C***** REF. - LINEAR INTERPOLATION OF GRAPHICAL RESULTS  
C***** PRESENTED BY HOTTEL - DATA AND CALC. PROCEDURE  
C***** PP. 228 & 234  
C***** PL - TOTAL RADIATING COMPONENT MOLE FRACTION  
C***** MULTIPLIED BY THE BEAM LENGTH (0.9*DIAMETER)  
C***** RADCT(I) = 1 FOR RADIATING GAS,  
C***** = 0 FOR NON-RADIATING GAS
```

```
TMENR=TMEAN+459.69
```

```
PL=0.
```

```
DO 3 I=1,NGMS
```

```
3 PL=PL+RADCT(I)*YAVG(I)
```

```
PL=PL*(PRESS/14.696/YTOT)*(TDIAM/12.0)*0.90
```

```
EMIS=0.
```

```
C***** FIND ORDINATE BY LINEAR INTERPOLATION
```

```
6 DO 4 K=2,4
```

```
IF(ALOG(PL)-RPL(K)) 5,5,4
```

```
4 CONTINUE
```

```
5 ORD= (ALOG(PL)-RPL(K-1))*(EPS(K)-EPS(K-1))/(RPL(K)  
$-RPL(K-1))
```

```
C***** CHECK TO SEE IF GAS EMISSIVITY HAS BEEN CALCULATED
```

```
IF(EMIS-1.0E-10) 7,7,8
```

```
C***** CALCULATE GAS EMISSIVITY FROM GRAPHICAL ORDINATE
```


SUBROUTINE HLOSS ...(CONT'D)

```
7 EMIS=EXP(ORD+EPS(K-1))/TMENR
```

```
C***** SAVE PL(EMIS) , AND CONVERT PL FOR CALCULATION OF
C***** ABSORPTIVITY OF GAS AT WALL TEMP, THEN RETURN TO
C***** 6 FOR CALCULATION OF NEW VALUE OF ORD
```

```
PL1=PL
PL=PL*(TWALL+459.69)/TMENR
GO TO 6
```

```
C***** CALCULATE GAS ABSORPTIVITY FROM GRAPHICAL ORDINATE
```

```
8 ABSOR=(EXP(ORD+EPS(K-1))/TMENR)*(TMENR/(TWALL+459.69))
  **0.5
```

```
IF(ITEST-7) 807,806,806
806 WRITE(IWRIT,5005) PL1,EMIS,PL,ABSOR
807 CONTINUE
```

```
QGRAD=(EPSP+1)/2.*(EMIS*(TMEAN+459.69)**4-ABSOR*(TWALL+
1 459.69)**4)*0.1713E-8*AREA
```

```
C***** CALCULATE TOTAL HEAT LOSS.
```

```
20 CONTINUE
```

```
QLOSS=QLOSS+QCONV+QGRAD
IF(ITEST-6) 805,804,804
804 WRITE(IWRIT,5002) CPAVG,AREA,HG,UCONV,DTLM
805 CONTINUE
IF(ITEST-5) 801,800,800
800 WRITE(IWRIT,5000) GT,TNUMB,TDIAM,DELPC,QCONV,QGRAD
  $,QLOSS,TFEED,TEMP
801 CONTINUE
RETURN
```

```
5000 FORMAT(1H0,' GT = ',E15.7,5X,' TNUMB = ',E15.7,5X
  $,' TDIAM = ',E15
  1.7,5X,/' DELPC = ',E15.7,5X,' QCONV = ',E15.7,5X,' QGRAD
  $ = ',E15.7/
  1' QLOSS = ',E15.7,5X,' TFEED = ',E15.7,5X,' TEMP = '
  $,E15.7)
5002 FORMAT(1H0,' CPAVG = ',E15.7,2X,' AREA = '
  $,E15.7,2X,
  1' HG = ',E15.7,/1X,' UCONV = ',E15.7,2X,' DTLM = '
  $,E15.7,2X)
5005 FORMAT(1H0,' PL1 = ',E15.7,2X,' EMIS = '
  $,E15.7,2X,
  1' PL = ',E15.7,/1X,' ABSOR = ',E15.7)
END
```



```

C *****
C *
C *          SUBROUTINE PDROP
C *
C * FUNCTIONS -
C *
C * - BOILER TUBE PASS PRESSURE DROP CALCULATION
C * ROUTINE
C * - CALCULATES PRESSURE DROP IF TUBE DIAMETER
C * SPECIFIED (IFLAG=1)
C * - FINDS MINIMUM VALID TUBE DIAMETER (FOR GIVEN
C * TUBE NUMBER) WHICH WILL RESULT IN LESS THAN
C * SPECIFIED MAXIMUM ALLOWABLE PRESSURE DROP
C * (IFLAG=2)
C * - FOR (IFLAG=2), STOPS ALTERNATION BETWEEN TWO
C * DIAMETERS IF ALTERNATING SHOULD OCCUR
C *
C *****

```

```

SUBROUTINE PDROP(AVG MU,WAL MU,RHO,TMASS,GT,ITERH)
DIMENSION DVALD(15)
COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /HTLS1/TNUMB,TDIAM,TLONG,TSHL1,TSHL2,QLOSS
$,DELPC,DELTP
COMMON /BURN2/IFLAG,IPASS,MPASS,ESTMT(3)
DATA DVALD/0.5,0.75,1.,1.5,2.,2.5,3.,4.,6.,8.,10.,12.
$,16.,18.,20./

```

```

C***** NON-ADIABATIC - EITHER DESIGN OR SIMULATION
C***** CALCULATE PRESSURE DROP THROUGH TUBE PASS.
C***** FOR SIMULATION CASE, CALCULATE DELPC DIRECTLY (NO
C***** ITERATION).
C***** FOR DESIGN CASE, TRY VALID PIPE DIAMETERS (DVALD)
C***** UNTIL THE MAXIMUM PRESS. DROP SPEC. IS MET.

```

```

TDOLD=TDIAM
DO 1 IJK=1,15
IF(IFLAG-1) 2,2,3
3 TDIAM=DVALD(IJK)
2 PHI=(AVG MU/WAL MU)**0.14
A1=5.0*TLONG/(TDIAM*RHO)
A2=0.0416*TDIAM/TLONG

```

```

C***** CALCULATE MASS VELOCITY

```

```

GT=TMASS/(TNUMB*3.14159*TDIAM**2/4)*144.

```

```

C***** CALCULATE REYNOLD'S NUMBER

```

```

PE=0.0344*TDIAM*GT/AVG MU

```

```

C***** CALCULATE FRICTION FACTOR USING BLASIU'S EQN.

```


SUBROUTINE PDROP ... (CONT'D)

$$FF = 0.079 / RE^{0.25}$$

C***** CALCULATE PRESSURE DROP USING TEMA EXPRESSION

DELPC=A1*(FF/PHI+A2)*(GT/1.0E+5)**2

IF(IFLAG-1) 4,4,5

5 IF(ITEST-10) 803,802,802

802 WRITE(IWRIT,5001) GT,RE,FF,TDIAM,A1,A2,PHI,DELPC

803 CONTINUE

IF((DELPC-DELTP)/DELTP-CRIT**0.333333) 4,4,1

1 CONTINUE

4 IF(ITEST-5) 805,804,804

804 WRITE(IWRIT,5001) GT,RE,FF,TDIAM,A1,A2,PHI,DELPC

805 CONTINUE

IF(ITERH-6) 50,50,51

51 IF(TDOLD-TDIAM) 50,50,52

52 TDIAM=TDOLD

GO TO 2

50 RETURN

5001 FORMAT(1H0,'INTERMEDIATE RESULTS'/) GT = ',E15.7,2X

\$,

1' RE = ',E15.7,2X,' FF = ',E15.7,2X,/' TDIAM = '

\$,E15.7,2X,

1' A1 = ',E15.7,2X,' A2 = ',E15.7,2X,/' PHI = '

\$,E15.7,2X,

1' DELPC = ',E15.7)

END


```

C *****
C *
C *          SUBROUTINE INLNB
C *
C * FUNCTIONS -
C *
C * - PRIMARY IN-LINE BURNER ROUTINE
C * - INITIALIZES CALCULATIONS -- THEN DESIGNS OR
C *   SIMULATES AN IN-LINE BURNER
C * - DEFINES EQUIPMENT FEED AND PRODUCT STREAMS
C *
C *****

```

```

      SUBROUTINE INLNB
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /BURN1/TCTOF,TBURN,IMUFF,NLGTH,NDIAM,NRTIM
      $,NHRLS,NBURN
      WRITE(IWRIT,6000) NMBEQ

```

```

C*****      DEFINE COMBUSTION FEED.

```

```

      NSTRM=0
      CALL SUTIL(NSTRM,0,YFEED,TFEED,PRESS)
      CALL PRNTS(-1)

```

```

C*****      DESIGN/SIMULATE COMBUSTION CHAMBER.

```

```

      TCTOF=+1.0
      IMUFF=-1
      NBURN=ILOC+5
      NLGTH=ILOC+1
      NDIAM=ILOC+2
      NRTIM=ILOC+3
      NHRLS=ILOC+4
      CALL BRXNC

```

```

C*****      DEFINE EQUIPMENT OUTLET STREAM.

```

```

      NEXIT=NSOUT(1)
      CALL SUTIL(NEXIT,2,YCOMP,TEMP,PRESS)
      IF(ITEST-1) 801,800,800
800  WRITE(IWRIT,6001)
      CALL PRNTS(NEXIT)
801  CONTINUE
      RETURN
6000  FORMAT(T48,'INLINE BURNER.'/T45,'EQUIPMENT NUMBER '
      $,I3)
6001  FORMAT('1'////T45,'BURNER EXIT STREAM -')
      END

```



```

C  ****
C  *
C  *          SUBROUTINE BRNXC
C  *
C  *  FUNCTIONS -
C  *
C  *  -  BURNER REACTION CHAMBER UTILITY ROUTINE
C  *  -  DESIGNS OR SIMULATES A COMBUSTION CHAMBER
C  *      {IN-LINE BURNER, BOILER MUFFLE FURNACE OR
C  *      BOILER FIRE TUNNEL}
C  *  -  FINDS ADIABATIC FLAME TEMPERATURE OF REACTION
C  *  -  DESIGN CASE -- FINDS SUITABLE COMBUSTION
C  *      CHAMBER LENGTH AND DIAMETER
C  *  -  SIMULATION CASE -- FINDS REACTION RESIDENCE
C  *      TIME AND UNIT VOLUME HEAT RELEASE
C  *
C  ****

```

```

      SUBROUTINE BRXNC
      REAL LENGTH
      DIMENSION XVALD(7),DVALD(10)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /STOR1/EQUIP(300),ILOD,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /BURN1/TCTOF,TBURN,IMUFF,NLGTH,NDIAM,NRTIM
      $,NHRLS,NBURN
      DATA NOXS,XVALD/7,10.,16.,20.,24.,30.,40.,50./
      DATA NODS,DVALD/10,6.,8.,10.,12.,18.,24.,36.,48.,60.
      $,72./
      DATA IFIRST/0/
      IF(IFIRST) 80,80,81
      80 TBURN=2000.0
      IFIRST=1
      81 CONTINUE

```

```

C*****      CALCULATE ADIABATIC FLAME TEMP.

```

```

      DO 100 I=1,NTOT
      100 YCOMP(I)=YFEED(I)

```

```

C*****      TBURN PREVIOUSLY CALCULATED, ESTIMATED, OR GUESSED
C*****      2000. F.

```

```

      TBURN=SETVU(EQUIP(NBURN),TBURN)
      TEMP=TBURN
      NOHLS=0
      CALL TCALC(NOHLS)
      TBURN=TEMP
      IF(IMUFF)300,301,301
      300 IF(ITEST-1) 803,802,802
      802 WRITE(IWRIT,9000)

```


SUBROUTINE BRNXC ... (CONT'D)

```

803 CONTINUE
  GO TO 302
301 CALL PRNTS(0)
302 CONTINUE

```

```

C*****  STORE ADIABATIC FLAME TEMPERATURE.

```

```

  EQUIP(NBURN)=TBURN

```

```

C*****  CALCULATE TOTAL REACTION HEAT RELEASE.

```

```

  THRLS=ENTH-HFCAL(TFEED,YCOMP,0)

```

```

C*****  SET NEW FEED TO RXN. PROD.

```

```

  TFEED=TEMP
  YTOT=0.0
  DO 103 I=1,NGMS
    YTOT=YTOT+YCOMP(I)
103 YFEED(I)=YCOMP(I)
  ISIM=1

```

```

C*****  DESIGN OR SIMULATION.

```

```

C*****  HERE TO 30 - DESIGN OF REACTION CHAMBER - HRELS
C*****  AND/OR RTIME SPECIFIED, CHAMBER DIMENSIONS
C*****  CALCULATED.

```

```

  VOLUM=0.0

```

```

C*****  IF RTIME SPECIFIED, CALC. RXN. VOLUME.

```

```

  IF(EQUIP( NRTIM )) 20,22,22
20 RTIME =-EQUIP( NRTIM )
  VOLUM=RTIME*10.73*(TEMP+459.69)*YTOT/3600./PRESS

```

```

C*****  IF HRELS SPECIFIED, CALC. RXN. VOLUME.

```

```

  22 IF(EQUIP( NHRLS )) 21,23,23

```

```

C*****  IF NEITHER GIVEN, MUST BE SIMULATION CASE.

```

```

  23 IF(VOLUM-1.0E-2) 30,30,25
  21 HRELS=-EQUIP( NHRLS )
  TESTV=THRLS/HRELS

```

```

C*****  IF BOTH ABOVE SPECIFIED, CHOOSE MAX. VOLUME.

```

```

  IF(TESTV-VOLUM) 25,25,24
  24 VOLUM=TESTV
  25 CONTINUE

```


SUBROUTINE BRNXC ... (CONT'D)

ISIM=0

```

C*****  CALCULATE RXN. CHAMBER DIMENSIONS.
C*****  FIND A VALID TUBE LENGTH AND DIAMETER.
C*****  (LENGTH/DIAMETER RATIO ABOUT 4.0)

```

$$LNGTH = (VOLUM * 64. / 3.14159) ** (1./3.)$$

```

C*****  FIND A SUITABLE LENGTH.

```

```

      DO 50 I=1,NOXS
      IF(XVALD(I)-LNGTH) 50,51,51
51  LNGTH=XVALD(I)
      GO TO 52
50  CONTINUE
      LNGTH=XVALD(NOXS)
52  DIAM=12.*(VOLUM*4./((3.14159*LNGTH)**0.5)

```

```

C*****  FIND A SUITABLE DIAMETER TO YIELD NECESSARY
C*****  VOLUME.

```

```

      DO 53 I=1,NODS
      IF(DVALD(I)-DIAM) 53,54,54
54  DIAM=DVALD(I)
      GO TO 55
53  CONTINUE
      DIAM=DVALD(NODS)
55  CONTINUE

```

```

C*****  EQUATE APPROPRIATE EQUIP. PARAMETERS TO FOUND
C*****  DIMENSIONS.

```

```

      EQUIP(NLGTH)=LNGTH
      EQUIP(NDIAM)=DIAM

```

```

C*****  FIND ACTUAL VOLUME, RTIME AND HRELS.

```

```

      GO TO 36

```

```

C*****  HERE TO END - SIMULATION OF REACTION CHAMBER -
C*****  DIMENSIONS SPECIFIED, CALCULATE RTIME AND HRELS

```

```

30  CONTINUE

```

```

C*****  EQUATE LNGTH AND DIAM TO SPECIFIED DIMENSIONS.

```

```

      LNGTH=SETVU(ABS(EQUIP(NLGTH)),20.)
      DIAM=SETVU(ABS(EQUIP(NDIAM)),60.)

```

```

C*****  CALCULATE RTIME AND HRELS.

```


SUBROUTINE BRNXC ... (CONT'D)

```

36  VOLUM=3.14159*(DIAM/12.)**2.*LNGTH/4.
    HRELS=THRLS/VOLUM
    RTIME=VOLUM*3600.*PRESS/10.73/(TEMP+459.69)/YTOT
    EQUIP(NRTIM)=SIGN(RTIME,EQUIP(NRTIM))
    EQUIP(NHRLS)=SIGN(HRELS,EQUIP(NHRLS))
    IF(ITEST-1) 801,800,800
800  IF(IMUFF) 201,202,203
201  WRITE(IWRIT,2001)
    GO TO 204
202  WRITE(IWRIT,2002)
    GO TO 204
203  WRITE(IWRIT,2003)
204  IF (ISIM) 205,205,206
205  WRITE(IWRIT,2005)
    GO TO 207
206  WRITE(IWRIT,2006)
207  WRITE(IWRIT,2007) DIAM,RTIME,LNGTH,HRELS
    WRITE(IWRIT,9000)
801  RETURN
2001 FORMAT('+',T25,'IN-LINE BURNER -')
2002 FORMAT('+',T25,'BOILER FIRE TUNNEL -')
2003 FORMAT('+',T25,'MUFFLE FURNACE -')
2005 FORMAT(' ',T77,'(DESIGN)'/)
2006 FORMAT(' ',T73,'(SIMULATION)'/)
2007 FORMAT(T25,'DIAMETER (IN.) = ',F6.1,T54,'RESIDENCE
$ TIME (SEC.) = '
1,F7.3,/T25,'LENGTH (FT.) = ',F6.1,T50,'HEAT RELEASE
$ (BTU/CU.FT.) =
1 ',F7.0)
9000 FORMAT('0',T25,'*****')
$*****
1*****'/ )
END

```



```

C *****
C *
C *          SUBROUTINE CNVTR
C *
C * FUNCTIONS -
C *
C * - PRIMARY SULPHUR CONVERTER ROUTINE
C * - INITIALIZES CALCULATIONS -- DEFINES FEED AND
C *   DESIGNS OR SIMULATES CONVERTER BED
C * - DOES ADIABATIC REACTION TEMPERATURE CALCULATION
C * - CHECKS DEW POINTS WITHIN THE CONVERTER BED
C * - DEFINES OUTLET STREAM
C *
C *****

```

```

      SUBROUTINE CNVTR
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      COMMON /GEN2/TEMP, TFEED, YCOMP(20), YFEED(20), PRESS, ENTH
      COMMON /STOR1/EQUIP(300), ILOC, NMBEQ, STREM(50,22)
      $, NSIN(5), NSOUT(5)
      COMMON /BURN1/TCTOF, TBURN, IMUFF, NLGTH, NDIAM, NRTIM
      $, NHRLS, NBURN
      NUMBC=ABS(EQUIP(ILOC+1))
      WRITE(IWRIT,6000) NUMBC, NMBEQ

```

```

C*****      DEFINE CONVERTER FEED.

```

```

      NSTRM=0
      CALL SUTIL(NSTRM,0,YFEED,TFEED,PRESS)
      CALL PRCNT(1)
      CALL PRNTS(-1)

```

```

C*****      DESIGN/SIMULATE CONVERTER BED.

```

```

      CALL CRBED (DELTP)

```

```

C*****      CALCULATE EQUILIBRIUM OUTLET STREAM TEMP.

```

```

      DO 1 I=1,NTOT
1  YCOMP(I)=YFEED(I)
      TEMP=TFEED
      PRESS=PRESS-DELTP
      TCTOF=1.0
      NOHLS=0
      CALL TCALC(NOHLS)
      IF(ITEST-1) 803,802,802
802 WRITE(IWRIT,9000)
      WRITE(IWRIT,9001)
803 CONTINUE

```

```

C*****      CHECK DEW POINTS WITHIN CONVERTER BED.

```


SUBROUTINE CNVTR ... (CONT'D)

```
CALL DEWCK (DELTP)
CALL PRCNT(2)
```

```
C*****   DEFINE OUTLET STREAM
```

```
      NEXIT=NSOUT(1)
      CALL SUTIL(NEXIT,2,YCOMP,TEMP,PRESS)
      IF(ITEST-1) 801,800,800
800  WRITE(IWRIT,6001)
      CALL PRNTS (NEXIT)
801  CONTINUE
      RETURN
6000  FORMAT(T49,'CONVERTER ',I2/T45,'EQUIPMENT NUMBER 'I3)
6001  FORMAT(T43,'CONVERTER EXIT STREAM -')
9000  FORMAT('0',T25,'*****')
      $*****
      1*****'/)
9001  FORMAT('1')
      END
```



```

C *****
C *
C *          SUBROUTINE CRBED
C *
C * FUNCTIONS -
C *
C * - CONVERTER BED UTILITY ROUTINE
C * - CALCULATES TOTAL MASS, MOLES, AND GAS VOLUME
C * - DESIGN -- DETERMINES REQUIRED CROSS-SECTIONAL
C *   AREA AND DEPTH OF BED
C * - SIMULATION -- CALCULATES MOLAR FLOWRATE
C *   AND SUPERFICIAL VELOCITY THROUGH THE BED
C * - BOTH CASES -- CALCULATES PRESSURE DROP ACROSS
C *   THE BED
C *
C *****

```

```

SUBROUTINE CRBED (DELTP)
COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
$,NSIN(5),NSOUT(5)
COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)

```

```

C*****      FIND TOTAL STREAM MASS, MOLES AND GAS VOLUME.
C*****      (HOURLY BASIS)

```

```

      YTOT=0.0
      TMASS=0.0
      DO 1 I=1,NTOT
      YTOT=YTOT+YFEED(I)
      TMASS=TMASS+YFEED(I)*WTMOL(I)
1 CONTINUE
      P=PRESS-0.2
      T=TFEED+25.0+459.69
      VGAS=10.73*T*YTOT/P

```

```

C*****      DECIDE IF DESIGN OR SIMULATION.

```

```

      IF(EQUIP(ILOC+2)) 2,4,4
2 IF(EQUIP(ILOC+3)) 3,4,4

```

```

C*****      SIMULATION - BED XSECTIONAL AREA AND DEPTH GIVEN.

```

```

3 ISIM=1
      XAREA=-EQUIP(ILOC+2)
      DEPTH=-EQUIP(ILOC+3)
      VOLUM=XAREA*DEPTH

```

```

C*****      CALCULATE MOLAL FLOW RATE AND LINEAR VELOCITY THRU
C*****      BED.

```


SUBROUTINE CRBED ... (CONT'D)

```

FLOWR=YTOT/VOLUM
VELMX=VGAS/XAREA/3600.
GO TO 10

```

```

C***** DESIGN - FIND XAREA AND DEPTH.

```

```

4 ISIM=0

```

```

C***** VELMX SPECIFIED OR SET TO 1 FT/SEC.

```

```

VELMX=SETVU(-EQUIP(ILOC+6),1.0)

```

```

C***** FLOWR SPECIFIED OR SET TO 3 LB.MOLE/HR.CU.FT.

```

```

FLOWR=SETVU(-EQUIP(ILOC+7),3.0)

```

```

C***** CALCULATE NECESSARY VOLUME, XAREA AND DEPTH.

```

```

VOLUM=YTOT/FLOWR
XAREA=VGAS/VELMX/3600.
DEPTH=VOLUM/XAREA

```

```

C***** CHECK THAT BED IS AT LEAST 3 FEET THICK.

```

```

IF(DEPTH-3.0) 5,10,10
5 DEPTH=3.0
VOLUM=DEPTH*XAREA
FLOWR=YTOT/VOLUM

```

```

C***** CALCULATE PRESSURE DROP.

```

```

C***** PARTICLE DIAMETER SPECIFIED OR SET TO 0.5 IN.

```

```

10 PDIAM=SETVU(ABS(EQUIP(ILOC+8)),0.5)
DELTP=8.32*DEPTH*(TMASS/3600./XAREA)**2/PDIAM

```

```

C***** STORE VALUES.

```

```

EQUIP(ILOC+2)=SIGN(XAREA,EQUIP(ILOC+2))
EQUIP(ILOC+3)=SIGN(DEPTH,EQUIP(ILOC+3))
EQUIP(ILOC+4)=VOLUM
EQUIP(ILOC+5)=SIGN(DELTP,EQUIP(ILOC+5))
EQUIP(ILOC+6)=SIGN(VELMX,EQUIP(ILOC+6))
EQUIP(ILOC+7)=SIGN(FLOWR,EQUIP(ILOC+7))
EQUIP(ILOC+8)=SIGN(PDIAM,EQUIP(ILOC+8))
IF(ITEST-1) 801,800,800
800 IF(ISIM) 802,802,803
802 WRITE(IWRIT,1000)
GO TO 804
803 WRITE(IWRIT,1001)
804 WRITE(IWRIT,1002) XAREA,DEPTH,VOLUM,VELMX,FLOWR,PDIAM

```


SUBROUTINE CRBED ... (CONT'D)

```

$,DELTP
WRITE(IWRIT,9000)
801 CONTINUE
RETURN
1000 FORMAT(T25,'CONVERTER BED',T77,'(DESIGN)'/)
1001 FORMAT(T25,'CONVERTER BED',T73,'(SIMULATION)'/)
1002 FORMAT(T33'CROSSECTIONAL AREA (SQ.FT) = ',T69,F8.2,
$/T33'THICKNESS
1(FT.) = 'T69,F8.2 /T33,'VOLUME (CU.FT.) = 'T69,F8.2
$/T33'LINEAR GAS V
1ELOCITY (FT./SEC.) = 'T69,F8.2/T33'MOLAL FLOW RATE
$ (MOLE/HR.SQ.FT.)
1 = 'T69,F8.2/ T33'AVERAGE PARTICLE DIAMETER (IN.) = 'T69
$,F8.2/T33'PR
1ESSURE DROP (PSI.) = 'T69,F8.3)
9000 FORMAT('0',T25,'*****')
$*****
1*****'/)
END

```



```

C *****
C *
C *          SUBROUTINE DEWCK
C *
C *  FUNCTIONS -
C *
C *  -  SULPHUR DEW POINT CHECK ROUTINE
C *  -  DIVIDES CONVERTER BED TEMPERATURE RISE INTO
C *      INTERVALS -- DOES SULPHUR SHIFT AND THEN
C *      CALCULATES DEW POINT AT EACH INTERVAL --
C *      CHECKS THAT IT IS BELOW BED TEMPERATURE
C *  -  ASSUMES THAT CONVERSION REACTION IS LINEAR
C *      WITH TEMPERATURE ACROSS THE REACTION ZONE OF
C *      THE BED
C *
C *****

```

```

SUBROUTINE DEWCK (DELTP)

```

```

  DIMENSION YINCR(20)

```

```

  COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT

```

```

  COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH

```

```

C*****      CALCULATE DEW POINT TEMPERATURE AT 5 EQUAL TEMP.
C*****      INTERVALS BETWEEN THE INLET AND OUTLET CONVERTER
C*****      TEMPERATURES. ASSUME CONVERSION VARIES
C*****      PROPORTIONATELY WITH TEMPERATURE.

```

```

      IF(ITEST-2) 811,810,810
810 WRITE(IWRIT,999)
811 CONTINUE

```

```

C*****      SET TEMPERATURE, COMPOSITION AND PRESSURE
C*****      INCREMENTS.

```

```

      TINCR=(TEMP-TFEED)/5.0
      PINCR=DELTP/5.0
      DO 1 I=1,NTOT
1 YINCR(I)=(YCOMP(I)-YFEED(I))/5.0
      KINIT=0
      ISULF=1
      TDEWS=TEMP
      PRESS=PRESS+DELTP
      DO 2 J=1,5

```

```

C*****      FOR EACH INTERVAL, SET TEMP., COMPOSITION AND
C*****      PRESS.

```

```

      TEMP=TFEED+J*TINCR
      DO 3 I=1,NTOT
3 YCOMP(I)=YFEED(I)+J*YINCR(I)
      PRESS=PRESS-PINCR

```


SUBROUTINE DEWCK ...{CONT'D}

C***** DO SULPHUR SHIFT CALCULATION.

CALL SHIFT (KINIT,NTOT)

C***** DO DEW POINT TEMPERATURE (SULPHUR) CALCULATION.

CALL DEWPT(TDEWS,YCOMP,PRESS,ISULF)

C***** IF DIFFERENCE BETWEEN DEW POINT AND TEMP. SMALL,
C***** GIVE MESSAGE.

TDIFF=TEMP-TDEWS

IF(TDIFF-25.0) 10,11,11

10 WRITE(IWRIT,1001)

GO TO 800

11 IF(ITEST-2) 801,800,800

800 WRITE(IWRIT,1000) TEMP,TDEWS,TDIFF,PRESS

801 CONTINUE

2 CONTINUE

IF(ITEST-2) 803,802,802

802 WRITE(IWRIT,9000)

803 CONTINUE

RETURN

999 FORMAT(////T41'CONVERTER DEW POINT CHECK -'//

1T25' BED DEW POINT TEMPERATURE

\$ BED '//

1T25' TEMPERATURE TEMPERATURE DIFFERENCE

\$ PRESSURE '/')

1000 FORMAT(T28,4(F8.3,7X))

1001 FORMAT(T30,'TEMPERATURE IS LESS THAN 25 DEG.F ABOVE

\$ DEW POINT.')

9000 FORMAT('0',T25,'*****')

\$*****

1*****')

END


```

C *****
C *
C *          SUBROUTINE CONDR
C *
C * FUNCTIONS -
C *
C * - PRIMARY SULPHUR CONDENSER ROUTINE
C * - INITIALIZES CALCULATIONS -- DEFINES CONDENSER
C *   FEED AND CALCULATES TOTAL INLET SULPHUR
C * - DEFINES GAS AND SULPHUR OUTLET STREAMS AND
C *   STEAM STREAMS IF PRESENT
C * - CHECKS DATA COMPATIBILITY
C * - 'INTEGRATES' DOWN THE CONDENSER
C * - CALCULATES RESULTING OVERALL HEAT TRANSFER
C *   COEFFICIENT, STEAM PRODUCTION, AND OUTLET FOG
C *   IN GASEOUS CONDENSER OUTLET STREAM
C * - STORES CONDENSER OUTLET STREAMS.
C *
C *****

```

```

      SUBROUTINE CONDR
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      COMMON /GEN2/TEMP, TFFED, YCOMP(20), YFEED(20), PRESS, ENTH
      COMMON /STOR1/EQUIP(300), ILOC, NMBEQ, STREM(50,22)
      $, NSIN(5), NSOUT(5)
      COMMON /COND1/NTUBE, DIAM, IS8, ISUL, TSTEM, SMINR, SULIN
      $, YSULF(20)
      DATA TCOND/250.0/
      NUMBC=ABS(EQUIP(ILOC+1))+0.5
      WRITE(IWRIT,6000) NUMBC, NMBEQ

```

```

C*****      DEFINE FEED STREAM.

```

```

      NSTRM=0
      CALL SUTIL(NSTRM,0,YFEED,TFFED,PRESS)

```

```

C*****      FIND TOTAL MASS SULPHUR INTO CONDENSER.

```

```

      CALL SUMFR(YFEED,NTOT,1,DUMY,TMSIN)
      CALL PRNTS(-1)

```

```

C*****      DEFINE GAS OUTLET (NEXIT), SULPHUR OUTLET (NSULF)
C*****      STEAM SOURCE (NSTMS) AND PRODUCT (NSTMP) STREAMS.

```

```

      NSTMS=NSTRM
      NEXIT=NSOUT(1)
      NSTMP=IABS(NSOUT(3))
      NSULF=-EQUIP(ILOC+7)+0.5
      IF(NEXIT-NSULF) 2,1,2
1 NEXIT=NSOUT(2)

```

```

C*****      CHECK COMPATIBILITY OF STEAM PRESSURE AND OUTLET

```


SUBROUTINE CONDR ... (CONT'D)

C***** TEMP. DATA.

```
2 CALL COMPR(NSTMS,22,5)
  CALL COMPR(NSTMP,22,5)
  CALL COMPR(NEXIT,21,8)
```

C***** CALL CINIT TO INITIALIZE CONDENSER CALCULATIONS.

```
CALL CINIT (ISIM,TOUT,TLGTH,TINCR,NSTMS,PSTEM)
STREM(NEXIT,21)=EQUIP(ILOC+8)
DELT1=TFEED-TSTEM
```

C***** CALL CINTG TO DO CONDENSER 'INTEGRATION'

```
CALL CINTG(ISIM,TINCR,TLGTH,TOUT,TLONG,QTOTL,TCOND)
IF(ITEST-1) 801,800,800
800 IF(ISIM) 810,810,820
810 WRITE(IWRIT,1010)
  GO TO 803
820 WRITE(IWRIT,1020)
803 WRITE(IWRIT,9000)
  GMAX=ABS(EQUIP(ILOC+6))
  DELT2=TEMP-TSTEM
  AREA=NTUBE*3.14159*DIAM/12.0*TLONG
  UOVRL=QTOTL/((DELT1-DELT2)/ALOG(DELT1/DELT2)*AREA)
  WRITE(IWRIT,1000) TLONG,DIAM,NTUBE,GMAX,TEMP,UOVRL
  WRITE(IWRIT,9000)
801 CONTINUE
  CALL STEAM(QTOTL,TSTEM,PSTEM,NSTMS,NSTMP,5)
  CALL FOGST(TMSIN,NSULF,TCOND,NEXIT)
  CALL PRNTS(NEXIT)
  EQUIP(ILOC+2)=SIGN(TLONG,EQUIP(ILOC+2))
  EQUIP(ILOC+8)=SIGN(TEMP,EQUIP(ILOC+8))
  EQUIP(ILOC+12)=QTOTL
  RETURN
1000 FORMAT('0',T30,'TUBE LENGTH (FT.) =' ,T74,F6.1/T30'TUBE
  $ DIAMETER (I
  1N.) ='T74,F6.3/T30'NUMBER OF TUBES ='T76,I4/
  $/T30'MAXIMUM FLOW RATE
  1 (LB/SQ.FT.SEC) ='T74,F6.2/T30'OUTLET GAS TEMPERATURE
  $ (DEG.F) ='
  1T73,F7.1/T30'U (OVERALL) (BTU/HR.SQ.FT.DEG.F) ='T74
  $,F6.2)
1020 FORMAT('0',T45,'CONDENSER SIMULATION')
1010 FORMAT('0',T47,'CONDENSER DESIGN')
6000 FORMAT(T49'CONDENSER ',I2/T45,'EQUIPMENT NUMBER 'I3)
9000 FORMAT('0',T25,'*****
$*****
}*****')
END
```



```

C *****
C *
C *          SUBROUTINE CINIT
C *
C * FUNCTIONS -
C *
C * - CONDENSER INITIALIZATION ROUTINE
C * - SETS STEAM PRESSURE AND CALCULATES STEAM
C *   TEMPERATURE
C * - IDENTIFIES S8 AND LIQUID SULPHUR SPECIES
C * - INITIALIZES SULPHUR CONDENSATE FILM STREAM
C * - SETS CONDENSER TUBE DIAMETER
C * - DESIGN CASE -- DEFINES CONDENSER GAS OUTLET
C *   TEMPERATURE
C * - SIMULATION CASE -- DEFINES CONDENSER LENGTH
C * - EITHER CASE -- DEFINES NUMBER OF TUBES AND
C *   'INTEGRATION' TEMPERATURE INTERVAL
C *
C *****

```

```

SUBROUTINE CINIT (ISIM,TOUT,TLGTH,TINCR,NSTMS,PSTEM)
DIMENSION YSTEM(20)
COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
$,NSIN(5),NSOUT(5)
COMMON /COND1/NTUBE,DIAM,IS8,ISUL,TSTEM,SMINR,SULIN
$,YSULF(20)
COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)
COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)

```

```

C*****      SET STEAM PRESSURE (50.0 PSIA. IF NOT SPECIFIED),
C*****      AND CALCULATE SATURATION TEMPERATURE.

```

```

CALL SUTIL(NSTMS,1,YSTEM,TSTEM,PSTEM)
PSTEM=SETVU(-EQUIP(ILOC+5),50.0)
YSTEM(IDH2O)=1.0
TSTEM=SETVU(TSTEM,250.0)
CALL DEWPT(TSTEM,YSTEM,PSTEM,0)

```

```

C*****      HERE TO 11 - IDENTIFY S8 (IS8) AND S1(L) (ISUL).
C*****      DEFINE SULPHUR COLUMN IN FORMU MATRIX.

```

```

ICOL=IDATM(1)
ICHCK=0
DO 8 I=1,5
  IVALU=IDSUL(I)

```

```

C*****      IF SULPHUR SPECIF NO. G.T. NGMS ASSUME S1(L)

```

```

IF( IVALU-NGMS) 6,6,9

```


SUBROUTINE CINIT ... (CONT'D)

C***** CHECK FOR S8.

```

6 IF(ABS(FORMU(IVALU,ICOL)-8.0)-0.1) 7,7,8
7 IS8=IVALU
  ICHCK=ICHCK+1
  GO TO 8
9 ISUL=IVALU
  ICHCK=ICHCK+1
8 CONTINUE
  IF(ICHCK-2) 10,11,10
10 WRITE(IWRIT,5000)

```

```

5000 FORMAT('O ERROR W.R.T. PRESENCE OF S8 AND/OR S1(L)
$ SPECIES.')
```

11 CONTINUE

C***** INITIALIZE SULPHUR FILM STREAM (YSULF) TO ZERO.
C***** SET LIQ SULPHUR TO SMALL INITIAL VALUE.

```

DO 12 I=1,NTOT
12 YSULF(I)=0.0
  YSULF(ISUL)=1.0E-6

```

C***** SUM TOTAL MOLES AND TOTAL MASS INTO CONDENSER.

```
CALL SUMER(YFEED,NGMS,0,YTOT,TMASS)
```

C***** SET TUBE DIAMETER (1.0 IN. IF NOT SPECIFIED.)

```
DIAM=SETVU(-EQUIP(ILOC+3),1.0)
```

C***** CHECK IF TUBE LENGTH SPECIFIED. DECIDE IF
C***** SIMULATION OR DESIGN.

```

TLGTH=-EQUIP(ILOC+2)
IF(TLGTH) 100,100,200

```

C***** DESIGN CASE -
C***** SPECS SHOULD BE DIAM,GMAX AND TOUT (OR RECOV).
C***** CALCULATE TLGTH,NUMBT, AND RECOV

```
100 ISIM=0
```

C***** IF CONDENSER OUTLET TEMP. GIVEN, SET TOUT.

```

TOUT=-EQUIP(ILOC+8)
IF(TOUT) 101,101,110

```

C***** TEMP. NOT SPECIFIED. - SET RECOVERY. IF RECOVERY
C***** NOT SPECIFIED, ASSUME 90.0 PERCENT.
C***** FIND OUTLET TEMP. FOR GIVEN RECOVERY.

SUBROUTINE CINIT ... (CONT'D)

C***** (I.E. DEW POINT OF INLET STREAM MINUS SPECIFIED
 C***** SULPHUR RECOVERY).

101 RECOV=SETVU(-EQUIP(ILOC+9),95.0)/100.0
 ICNTS=1

DO 102 I=1,NTOT

YCOMP(I)=YFEED(I)

IF(I-IDISUL(ICNTS)) 102,103,102

103 ICNTS=ICNTS+1

YCOMP(I)=YCOMP(I)*(1.0-RECOV)

102 CONTINUE

TOUT=TFEED

CALL DEWPNT(TOUT,YCOMP,PRESS-0.3,1)

110 CONTINUE

C***** MAKE SURE OUTLET TEMP. (TOUT) IS ABOVE TSTEM.

IF(TOUT-(TSTEM+10.0))115,120,120

115 TOUT=TSTEM+10.0

120 CONTINUE

EQUIP(ILOC+8)=-TOUT

C***** SET TEMPERATURE INCREMENT.

TINCR=(TFEED-TOUT)/10.0

C***** SET MAXIMUM ALLOWABLE MASS FLOW RATE. (4.0

C***** LB./SQ.FT.SEC. IF NOT SPECIFIED.) AND CALCULATE

C***** REQUIRED CROSSECTIONAL TUBE AREA AND TUBE NUMBER.

GMAX=SETVU(-EQUIP(ILOC+6),4.0)

AREA=TMASS/(3600.*GMAX)

NTUBE=AREA*4.*144./(3.14159*DIAM**2)+0.5

GO TO 300

200 ISIM=1

C***** SIMULATION CASE -

C***** SPECS SHOULD BE DIAM,TLGTH, AND NUMBT.

C***** CALCULATE GMAX,TOUT AND RECOV.

NTUBE=-EQUIP(ILOC+4)+0.5

C***** IF NTUBE NOT SPECIFIED, REVERT TO DESIGN.

IF(NTUBE) 100,100,201

C***** SET TEMP. INCREMENT TO 5 DEG.F.

201 TINCR=25.0

TOUT=0.0

SUBROUTINE CINIT ...(CONT'D)

```

C***** CALCULATE ACTUAL AREA, MAX. FLOW RATE AND STORE
C***** SET VALUES.

300 AREA=NTUBE*3.14159*DIAM**2/(4.*144.)
   GMAX=TMASS/(3600.*AREA)
   EQUIP(ILOC+3)=SIGN(DIAM ,EQUIP(ILOC+3))
   TUBE=NTUBE
   EQUIP(ILOC+4)=SIGN(TUBE ,EQUIP(ILOC+4))
   EQUIP(ILOC+5)=SIGN(PSTEM,EQUIP(ILOC+5))
   EQUIP(ILOC+6)=SIGN(GMAX ,EQUIP(ILOC+6))
   IF(ITEST-4) 801,800,800
800 WRITE(IWRIT,1000) ISIM,TLGTH,TOUT,IS8,ISUL,NTUBE,DIAM
801 CONTINUE
   DO 400 I=1,NTOT
400 YCOMP(I)=YFEED(I)
   KINIT=1
   TEMP=TFEED
   CALL SHIFT(KINIT,NTOT)
   DO 401 I=1,NTOT
401 YFEED(I)=YCOMP(I)
   RETURN
1000 FORMAT('0',' ISIM ='I2, 2X'TLGTH ='E15.7,/
1'  TOUT ='E15.7,2X' IS8 ='I3 ,2X' ISUL ='I3 /
1' NTUBE ='I4 ,2X' DIAM ='E15.7)
   END

```



```

C *****
C *
C *          SUBROUTINE CINTG
C *
C *  FUNCTIONS -
C *
C *  -  CONDENSER 'INTEGRATION' ROUTINE
C *  -  INTEGRATES DOWN THE CONDENSER TUBES BY
C *      BREAKING THE CONDENSER INTO SEGMENTS DEFINED
C *      BY TEMPERATURES
C *  -  FOR EACH SEGMENT OUTLET TEMPERATURE, CALCULATES
C *      SULPHUR VAPOR PRESSURE AND MOLES OF SULPHUR AT
C *      SATURATION -- FINDS MINIMUM SULPHUR CONDENSATION
C *      FOR SEGMENT TO PREVENT SUPER-SATURATION AT OUTLET
C *  -  CALCULATES SEGMENT LENGTH AND PRESSURE DROP --
C *      DOES A SULPHUR SHIFT AT EACH SEGMENT OUTLET
C *  -  AT END OF CONDENSER (DEFINED BY TEMPERATURE FOR
C *      DESIGN OR LENGTH FOR SIMULATION) RATIOS
C *      PORTION OF LAST SEGMENT TO USE. (ASSUMES
C *      COMPOSITION, PRESSURE, TEMPERATURE AND HEAT LOSS
C *      ARE LINEAR WITH LENGTH OVER LAST SEGMENT)
C *
C *****

```

```

      SUBROUTINE CINTG(ISIM,TINCR,TLGTH,TOUT,TLONG,QTOTL
$,TCOND)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /COND1/NTUBE,DIAM,IS8,ISUL,TSTEM,SMINR,SULIN
$,YSULF(20)
      COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)
      DATA AREA /30.0/

```

```

C*****      INITIALIZE CONDENSER HEAT LOAD AND LENGTH TO ZERO.

```

```

      QTOTL=0.0
      DENTH=HFCAL(TFEED,YFEED,0)-ENTH
      TLONG=0.0
      IFINI=0

```

```

C*****      CONDENSER SEGMENT LOOP
C*****      EFFECTIVE INTEGRATION DOWN CONDENSER USING SMALL
C*****      TEMPERATURE INTERVALS (TINCR).
C*****      SET SEGMENT OUTLET TEMP.

```

```

      500 TEMP=TFEED-TINCR

```

```

C*****      EVALUATE SULPHUR VAPOR PRESS. AT OUTLET TEMP.

```

```

      CALL VPRES(VPMAX,DVPDT,TEMP,1)
      VPMAX=VPMAX*14.696

```


SUBROUTINE CINTG ... (CONT'D)

C***** FIND SULPHUR AND TOTAL MOLES (GAS) INTO SEGMENT.

CALL SUMER(YFEED,NGMS,1,SULIN,SMASS)

CALL SUMER(YFEED,NGMS,0,YTOT,TMASS)

C***** FIND MAXIMUM SULPHUR MOLES IN SEGMENT OUTLET FOR

C***** SATURATED OUTLET (SMOLS), AND MINIMUM SULPHUR

C***** REMOVAL TO ACHIEVE THIS SATURATED OUTLET (SMINR).

YINRT=YTOT-SULIN

SMOLS=VPMAX*YINRT/(PRESS-VPMAX)

SMINR=SULIN-SMOLS

C***** IF SMINR +VE, SET OUTLET TO SATURATED CONDITION.

C***** (THIS IS ONLY AN ESTIMATE FOR THE OUTLET).

IF(SMINR) 509,509,505

509 SMINR=0.0

GO TO 510

505 ICNTS=1

DO 507 I=1,NTOT

IF(I-IDSUL(ICNTS)) 507,506,507

506 YCOMP(I)=YFEED(I)*SMOLS/SULIN

ICNTS=ICNTS+1

GO TO 508

507 YCOMP(I)=YFEED(I)

508 CONTINUE

510 CONTINUE

IF(ITEST-3) 801,800,800

800 WRITE(IWRIT,1000)TFEED,TEMP,VPMAX,SMOLS,SMINR,SULIN

801 CONTINUE

C***** STORE LIQUID SULPHUR.

SLIQ=YSULF(ISUL)

C***** CALL CSECT TO SOLVE FOR THE CONDENSER SECTION AREA

C***** , HEAT LOSS AND SEGMENT OUTLET GAS AND LIQUID

C***** STREAMS.

CALL CSECT(AREA,QLOSS,TCOND,DPPFT,DENTH)

C***** CALCULATE SEGMENT LENGTH AND PRESSURE DROP.

SGMTL=AREA/(NTUBE*3.14159*DIAM/12.)

DELTP=SGMTL*DPPFT

C***** HERE TO 850 - DECIDE IF INTEGRATION COMPLETE, AND

C***** UPDATE STREAM PARAMETERS.

SUBROUTINE CINTG ...(CONT'D)

```
RATIO=1.0
IF(ISIM) 750,750,700
```

```
C***** SIMULATION CASE - FINISHED IF CUMULATIVE SEGMENT
C***** LENGTH IS EQUAL OR GREATER THAN SPECIFIED
C***** CONDENSER LENGTH.
```

```
700 IF(TLONG+SGMTL-TLGTH) 760,702,702
```

```
C***** SET RATIO OF FINAL SEGMENT TO USE.
```

```
702 RATIO=1.0-(TLONG+SGMTL-TLGTH)/SGMTL
IFINI=1
GO TO 760
```

```
C***** DESIGN CASE - FINISHED IF SEGMENT OUTLET
C***** TEMPERATURE IS EQUAL OR LOWER THAN SPECIFIED
C***** CONDENSER OUTLET TEMP. (OR ALTERNATELY , OUTLET
C***** TEMP. REQUIRED FOR SPECIFIED CONDENSER RECOVERY.)
```

```
750 IF(TEMP-TOUT-0.1) 752,752,760
```

```
C***** SET RATIO OF FINAL SEGMENT TO USE.
```

```
752 RATIO=1.0+(TEMP-TOUT)/TINCR
IFINI=1
```

```
C***** DEFINE SEGMENT OUTLET PRESSURE,TEMPERATURE,AND
C***** CUMULATIVE CONDENSER TUBE LENGTH AND HEAT LOSS.
```

```
760 PRESS=PRESS-DELTP*RATIO
TEMP=TFEED-TINCR*RATIO
TLONG=TLONG+SGMTL*RATIO
QTOTL=QTOTL+QLOSS*RATIO
```

```
C***** CALL SHIFT TO DO EQUILIBRIUM SHIFT ON GASEOUS
C***** SULPHUR SPECIES.
```

```
KINIT=0
FNTH1=HFCAL(TEMP,YCOMP,0)
CALL SHIFT(KINIT,NGMS)
```

```
C***** SET OUTLET GAS STREAM COMPOSTTION AND NEW SEGMENT
C***** FEED AND TEMP. IN CASE MORE SEGMENTS REQUIRED.
```

```
ICNTS=1
DO 765 I=1,NTDT
IF(I-IDSUL(ICNTS)) 765,770,765
770 YCOMP(I)=YFEED(I)+(YCOMP(I)-YFEED(I))*RATIO
ICNTS=ICNTS+1
```


SUBROUTINE CINTG ... (CONT'D)

```
765 YFEED(I)=YCOMP(I)
    YSULF(ISUL)=SLIQ+(YSULF(ISUL)-SLIQ)*RATIO
    TFFED=TEMP
    DENTH=HFCAL(TEMP,YCOMP,0)-ENTH1
    IF(ITEST-3) 803,802,802
802 WRITE(IWRIT,1001) SGMTL,TLONG,QTOTL,DELTP,PRESS,RATIO,
    1 YSULF(ISUL),YCOMP(ISUL)
803 CONTINUE
```

C***** CHECK COMPLETION FLAG (IFINI).

```
    IF(IFINI) 500,500,900
900 QTOTL=QTOTL-DENTH
    RETURN
1000 FORMAT('0',
    1'TFEED ='E15.7,2X' TEMP ='E15.7,2X' VPMAX ='E15.7/
    1' SMOLS ='E15.7,2X' SMINR ='E15.7,2X' SULIN ='E15.7)
1001 FORMAT('0','SGMTL ='E15.7,2X'TLONG ='E15.7/
    1' QTOTL ='E15.7,2X'DELTP ='E15.7,2X'PRESS ='E15.7/
    1' RATIO ='E15.7,2X' SLIQ ='E15.7,2X' SFOG ='E15.7)
    END
```



```

C *****
C *
C *          SUBROUTINE CSECT
C *
C *  FUNCTIONS -
C *
C *  -  CONDENSER SEGMENT UTILITY ROUTINE
C *  -  FINDS CONDENSER SECTION AREA, HEAT LOSS AND
C *      OUTLET GAS (INCLUDING FOG FORMED) AND SULPHUR
C *      FILM STREAMS
C *  -  CALCULATES AVERAGE SEGMENT PROPERTIES,
C *      INCREMENTAL PRESSURE DROP, MOLECULAR VOLUME,
C *      DIFFUSIVITY AND GAS-SIDE HEAT TRANSFER
C *      COEFFICIENT
C *
C *****

```

```

      SUBROUTINE CSECT(AREA,QLLOSS,TCOND,DPPFT,DENTH)
      DIMENSION YAVG(20),VATOM(5)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /COND1/NTUBE,DIAM,IS8,ISUL,TSTEM,SMINR,SULIN
      $,YSULF(20)
      COMMON /DATA1/FORMU(20,5),NATYP,IDATM(5)
      COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)
      DATA TDEWS/350.0/

```

```

C*****      EVALUATE SOME STREAM PROPERTIES.

```

```

      CALL PROP(TDEWS,YAVG,AVGMU,WALMU,RHO,TMASS,YTOT,CPAVG)

```

```

C*****      CALCULATE MASS FLOW RATE THROUGH TUBES.

```

```

      GAVG=TMASS/(NTUBE*3.14159*DIAM**2/4)*144.

```

```

C*****      CONVERT VISCOSITY FROM CP. TO LB/FT.HR.

```

```

      VIS=AVGMU*2.42

```

```

C*****      CALCULATE INCREMENTAL PRESSURE DROP (PSI/FT.)

```

```

      RE=GAVG*DIAM/12/VIS

```

```

      FF=0.079/RE**0.25

```

```

      DPPFT=5*GAVG**2*FF/(DIAM*1.E10*RHO*(AVGMU/WALMU)**.14)

```

```

C*****      ESTIMATE THERMAL CONDUCTIVITY, USING HEAT CAPACITY
C*****      AND MOLECULAR WEIGHT. (REF. - PERRY)

```

```

      AVMWT=TMASS/YTOT

```

```

      RK=VIS*(CPAVG+2.48/AVMWT)

```

```

C*****      CALCULATE PRANDL NUMBER.

```


SUBROUTINE CSECT ... (CONT'D)

PR=CPAVG*VIS/RK

C***** HERE TO 5 - CALCULATE AVERAGE MOLECULAR WTS. OF
C***** SULPHUR GAS AND INERT GAS. CALCULATE WEIGHTED
C***** AVERAGE MOLECULAR VOLUMES.

CALL SUMER(YAVG,NGMS,1,SULFR,TSULF)
CALL SUMER(YAVG,NGMS,0,TOTAL,TMASS)
AMWTS=TSULF/SULFR
AMWTI=(TMASS-TSULF)/(TOTAL-SULFR)
VSULF=0.0
VINRT=0.0
ICNTS=1
DO 4 I=1,NGMS

C***** DECIDE IF PRESENT SPECIE SULPHUR VAPOR OR INERT.

IF(I-IDSUL(ICNTS)) 3,2,3
2 ICNTS=ICNTS+1
VSULF=VSULF+VMOLE(I)*YAVG(I)
GO TO 4
3 VINRT=VINRT+VMOLE(I)*YAVG(I)
4 CONTINUE
VSULF=VSULF/SULFR
TINRT=TOTAL-SULFR
VINRT=VINRT/TINRT
5 CONTINUE

C***** CALCULATE DIFFUSIVITY OF SULPHUR VAPOR IN INERT
C***** GAS. (SQ.FT./HR.) REF. - KERN.

TK32=((TFEED+TEMP)/2.0+459.69)/1.8)**1.5
DV=0.0166*TK32*(1/AMWTS+1/AMWTI)**0.5/(PRESS/14.696)
1 /(VSULF**0.3333+VINRT**0.3333)**2

C***** CALCULATE SCHMIDT AND REYNOLD NUMBERS, GAS SIDE
C***** HEAT TRANSFER COEFFICIENT, AND MASS TRANSFER
C***** COEFFICIENT FACTOR.

SC=VIS/(RHO*DV)
HG=0.023*RE**(-0.2)*CPAVG*GAVG/PR**0.6667
RKGFC=HG*PR**0.6667/(CPAVG*AVMWT*SC**0.6667)
IF(ITEST-4) 801,800,800
800 WRITE(IWRIT,1000) DPPFT,GAVG,RK,PR,AMWTS,VSULF,AMWTI,
1 VINRT,DV,SC,RE,HG
801 CONTINUE
CALL CHBAL(SULFR,TOTAL,RKGFC,AMWTS,CPAVG,HG,SULIQ,QA1
\$,TCOND)
CALL AQEND(TCOND,QA1,AMWTS,SULIQ,QLOSS,AREA,DENTH)
RETURN

SUBROUTINE CSECT ...[CONT'D]

```
1000 FORMAT('0','DPPFT ='E15.7,2X' GAVG ='E15.7,2X'   RK  
$ ='E15.7/  
1'      PR ='E15.7,2X'AMWTS ='E15.7,2X'VSULF ='E15.7/  
1' AMWTI ='E15.7,2X'VINRT ='E15.7,2X'   DV ='E15.7/  
1'      SC ='E15.7,2X'   RE ='E15.7,2X'   HG ='E15.7)  
END
```



```

C *****
C *
C *          SUBROUTINE CHBAL
C *
C * FUNCTIONS -
C *
C * - CONDENSATE FILM HEAT BALANCE ROUTINE
C * - ITERATIVELY ESTIMATES THE SEGMENT SULPHUR FILM
C *   TEMPERATURE SUCH THAT THE FILM HEAT BALANCE IS
C *   SATISFIED
C * - CALCULATES SULPHUR VAPOR PRESSURE AND LATENT
C *   HEAT OF VAPORIZATION AT FILM TEMPERATURE, MASS
C *   TRANSFER COEFFICIENT, HEAT LOSS FROM GAS TO
C *   FILM AND FROM FILM TO STEAM FOR EACH ESTIMATE
C *   OF FILM TEMPERATURE
C *
C *****

```

```

      SUBROUTINE CHBAL(SULFR,TOTAL,RKGFC,AMWTS,CPAVG,HG
      $,SULIQ,QAL,TCOND)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFFED,YCOMP(20),YFFED(20),PRESS,ENTH
      COMMON /COND1/NTUBE,DIAM,IS8,ISUL,TSTEM,SMINR,SULIN
      $,YSULF(20)

```

```

C*****      FIND CONDENSATE TEMPERATURE, TCOND, SUCH THAT HEAT
C*****      TRANSFER TO COND. FILM EQUALS THAT FROM IT.

```

```

      ITERH=0
      FAC1=1.1
      FAC2=1.0

```

```

      10 CALL GUESR(TCOND,FAC1,FAC2,ERROR,ITERH)

```

```

C*****      CALCULATE SULPHUR VAPOR PRESS. AT TCOND., AND
C*****      PARTIAL PRESSURE OF SULPHUR IN GAS.

```

```

      CALL VPRES(VPSUL,DVPDT,TCOND,1)
      VPSUL=VPSUL*14.696
      PPSUL=PRESS*SULFR/TOTAL

```

```

C*****      CALCULATE MASS TRANSFER COEFFICIENT.

```

```

      PGF=(PPSUL-VPSUL)/ALOG((PRESS-VPSUL)/(PRESS-PPSUL))
      RKG=RKGFC/PGF

```

```

C*****      CALCULATE LATENT HEAT OF VAPORIZATION (SULPHUR).

```

```

      HLIQ=HFCAL(TCOND,YSULF,0)
      YSULF(IS8)=YSULF(ISUL)
      HVAP=HFCAL(TCOND,YSULF,0)
      YSULF(IS8)=0.0
      DELTA=(HVAP-9*HLIQ)/(YSULF(ISUL)*256.)

```


SUBROUTINE CHBAL ... (CONT'D)

C***** CALCULATE MOLE FLUX SULPHUR TO CONDENSATE FILM.

SULIQ=RKG*(PPSUL-VPSUL)

C***** CALCULATE ACKERMANN COEFFICIENT (AC) TO ACCOUNT
C***** FOR EFFECT OF MASS TRANSFER ON HEAT TRANSFER.

A=SULIQ*AMWTS*CPAVG/HG
AC=A/(1.-EXP(-A))

C***** CALCULATE HEAT FLUX TO COND. FILM.

TMEAN=(TFEED+TEMP)/2.0
QA1=HG*(TMEAN-TCOND)*AC+SULIQ*DELTA*AMWTS

C***** CALCULATE FILM HEAT TRANSFER COEFFICIENT, HCOND.

TAU=YSULF(ISUL)*32.0/(NTUBE*3.14159*DIAM/12.)
RELIQ=TAU*0.1653
HCOND=327.9*RELIQ**(-0.3333)

C***** SPECIFY HEAT TRANSFER RESISTANCE FROM WALL, STEAM,
C***** AND FOULING.

RSCWF=0.006

C***** CALCULATE HEAT FLUX FROM COND. FILM TO STEAM.

UCTOS=1/(1/HCOND+RSCWF)
QA2=UCTOS*(TCOND-TSTEM)

C***** IF HEAT FLUXES EQUAL, CORRECT TEMPERATURE,
C***** OTHERWISE ITERATE ON TCOND.

ERROR=QA1-QA2
IF(ABS(ERROR/QA1)-CRIT**0.5) 11,11,10

11 CONTINUE

IF(ITEST-3) 804,802,802

802 WRITE(IWRIT,1002) ITERH,TCOND,QA1,QA2

IF(ITEST-4) 804,803,803

803 WRITE(IWRIT,1003) VPSUL,PPSUL,PGF,RKG,DELTA,SULIQ,AC
\$,HCOND

804 CONTINUE

RETURN

1002 FORMAT('0ITERH =' 'I3,2X' TCOND ='E15.7,2X' QA1 ='E15.7
\$,2X' QA2 ='E
115.7)

1003 FORMAT(' ', 'VPSUL ='E15.7,2X' PPSUL ='E15.7,2X' PGF
\$ ='E15.7/

SUBROUTINE CHRAL ... (CONT'D)

```
1'   RKG ='E15.7,2X'DELTA ='E15.7,2X'SULIQ ='E15.7/  
1'   AC  ='E15.7,2X'HCOND ='E15.7)  
END
```



```

C *****
C *
C * SUBROUTINE AQFND *
C *
C * FUNCTIONS - *
C *
C * - CONDENSER SEGMENT HEAT BALANCE ROUTINE *
C * - ITERATIVELY ESTIMATES THE SEGMENT LENGTH SUCH *
C * THAT A HEAT BALANCE ON THE SEGMENT IS SATISFIED *
C * - FOR EACH ESTIMATE OF LENGTH, THE SEGMENT MASS *
C * AND HEAT TRANSFER ARE CALCULATED -- THE SEGMENT *
C * OUTLET STREAMS ARE FOUND AND THEIR ENTHALPY IS *
C * CALCULATED *
C * - CHANGE IN SEGMENT STREAM ENTHALPIES MUST *
C * EQUAL SEGMENT HEAT LOSS *
C * - SEGMENT OUTLET MUST BE SATURATED OR SUPER-HEATED *
C * -- OTHERWISE FOG IS FORMED UNTIL SATURATION IS *
C * REACHED *
C *****

```

```

SUBROUTINE AQFND(TCOND, QAL, AMWTS, SULIQ, QLOSS, AREA
$, DENTH)
COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
COMMON /GEN2/TEMP, TFEED, YCOMP(20), YFEED(20), PRESS, ENTH
COMMON /COND1/NTUBE, DIAM, IS8, ISUL, TSTEM, SMINR, SULIN
$, YSULF(20)
COMMON /DATA5/IDH2O, IDSUL(5), WTMOL(20), VMOLE(20)

```

```

C***** ITERATIVELY CALCULATE INTER-DEPENDENT AREA AND
C***** HEAT LOSS.

```

```

C***** CALCULATE INLET ENTHALPY OF GAS AND LIQUID.

```

```

ENTH1=HFCAL(TFEED, YFEED, 0)+HFCAL(TCOND, YSULF, 0)

```

```

C***** STORE INLET LIQUID AND FOG SULPHUR.

```

```

SFOG=YCOMP(ISUL)
SLIQ=YSULF(ISUL)

```

```

C***** INITIALIZE GUESS ROUTINE PARAMETERS.

```

```

ITERH=0
FAC1=1.1
FAC2=1.0

```

```

C***** GENERATE A GUESS FOR AREA.

```

```

1 CALL GUESR(AREA, FAC1, FAC2, ERROR, ITERH)

```

```

C***** CALCULATE HEAT TRANSFER FOR THIS AREA.

```


SUBROUTINE AQEND ... (CONT'D)

QLOS1=AREA*QA1

C***** CALCULATE SULPHUR MOLES TRANSFERED FOR THIS AREA.

SMOLS=SULIQ*AREA

C***** HERE TO 25 - CALCULATE RESULTING OUTLET STREAMS.

IF(SMCLS-SMINR) 21,21,22

C***** OUTLET IS SATURATED OR SUPER-COOLED.

C***** IF SUPERCOOLED, FORM FOG TO BRING TO SATURATION.

21 SFACT=(SULIN-SMINR)/SULIN
YCOMP(ISUL)=SFOG+(SMINR-SMOLS)*AMWTS/32.0
GO TO 23

C***** OUTLET IS SUPER-HEATED.

22 SFACT=(SULIN-SMOLS)/SULIN
YCOMP(ISUL)=SFOG

C***** INCREASE CONDENSATE FILM BY MOLES TRANSFERED TO IT

23 YSULF(ISUL)=SLIQ+SMOLS*AMWTS/32.0

C***** DECREASE SULPHUR VAPOR BY THE APPROPRIATE AMOUNT.

DO 24 I=1,5
ICNTS=IDSUL(I)
IF(ICNTS-NGMS) 24,24,25
24 YCOMP(ICNTS)=YFEED(ICNTS)*SFACT
25 CONTINUE

C***** CALCULATE HEAT LOSS BY ENERGY BALANCE AROUND
C***** SECTION.

QLOSS=ENTH1-(HFCAL(TEMP,YCOMP,0)+HFCAL(TCOND,YSULF,0))
\$-DENTH

C***** ITERATE ON AREA IF IT HAS NOT CONVERGED.

C***** DEFINE ERROR AS HEAT LOSS DISCREPANCY.

ERROR=QLOS1-QLOSS
IF(ABS(ERROR/QLOSS)-CRIT) 27,27,1
27 CONTINUE
IF(ITEST-3) 807,805,805
805 WRITE(IWRIT,1004) ITERH,QLOSS,AREA,SMOLS
807 CONTINUE
RETURN

SUBROUTINE AQEND ... (CONT'D)

```
1004 FORMAT('OITERH ='I3,2X'QLOSS ='E15.7,2X' AREA ='E15.7  
$,2X'SMOLS ='E  
115.7)  
END
```



```

C *****
C *
C *          SUBROUTINE FOGST
C *
C *  FUNCTIONS -
C *
C *  - CONDENSER OUTLET FOG DETERMINATION ROUTINE
C *  - SETS OUTLET FOG TO SPECIFIED MAXIMUM IF THIS
C *    HAS BEEN SPECIFIED
C *  - CALCULATES CONDENSER PERCENTAGE CONDENSATION
C *    AND SULPHUR RECOVERY
C *  - STORES CONDENSER OUTLET STREAMS
C *
C *****

      SUBROUTINE FOGST(TMSIN,NSULF,TCOND,NEXIT)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /STOR1/EQUIP(300),ILOCC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      COMMON /COND1/NTUBE,DIAM,ISB,ISUL,TSTEM,SMINR,SULIN
      $,YSULF(20)
      IND=1
      IF(ITEST-1) 801,800,800
800 WRITE(IWRIT,1000)
801 CONTINUE

C*****    CALCULATE PERCENT OF INLET SULPHUR CONDENSED.

      1 SFOG=YCOMP(ISUL)
      WFOG=SFOG*32.0
      SLIQ=YSULF(ISUL)
      WLIQ=SLIQ*32.0
      CRCCOV=(WFOG+WLIQ)/TMSIN*100.0

C*****    FIND ACTUAL SULPHUR RECOVERY.

      ARCCOV=WLIQ/TMSIN*100.0
      IF(ITEST-1) 803,802,802
802 WRITE(IWRIT,2010) CRCCOV,ARCCOV
      WRITE(IWRIT,1002) SFOG,WFOG,SLIQ,WLIQ,NSULF,TCOND
      WRITE(IWRIT,9000)
803 CONTINUE
      IF(IND-1) 10,10,200

C*****    CHECK MAX SPECIFIED FOG FORMATION.

      10 FOGMX=-EQUIP(ILOCC+10)
      IF(FOGMX-0.1) 200,200,50
      50 CALL SUMER(YCOMP,NGMS,0,TOTAL,DUMY)
      CALL SUMER(YCOMP,NGMS,1,TOTS,DUMY)
      SDIFF=SFOG-(FOGMX*(TOTAL-TOTS)/(100.0*32.0))

```


SUBROUTINE FOGST ... (CONT'D)

```

      IF(SDIFF) 200,200,51
51  ENTH1=HFCAL(TCOND,YSULF,0)
      YSULF(ISUL)=SDIFF
      ENTHR=HFCAL(TEMP,YSULF,0)+ENTH1
      YSULF(ISUL)=SLIQ+SDIFF
      CALL FINDT(YSULF,TCOND,ENTHR)
      YCOMP(ISUL)=SFOG-SDIFF
      IF(ITEST-1) 809,804,804
804  WRITE(IWRIT,2000) FOGMX
      IF(FOGMX-20.0) 805,805,808
805  IF(FOGMX-4.0) 806,806,807
806  WRITE(IWRIT,2001)
      GO TO 810
807  WRITE(IWRIT,2002)
810  WRITE(IWRIT,2004)
808  WRITE(IWRIT,2003)
809  CONTINUE
      IND=2
      GO TO 1
200  CALL SUTIL(NEXIT,2,YCOMP,TEMP,PRESS)
      CALL SUTIL(NSULF,2,YSULF,TCOND,PRESS)
      EQUIP(ILOC+11)=ARCOV
      IF(ITEST-1) 812,811,811
811  WRITE(IWRIT,3001)
812  CONTINUE
      RETURN
1000  FORMAT('1'////T42'CALCULATED SULPHUR OUTLET')
1002  FORMAT('0'T31'SULPHUR FOG -      'F7.2' MOLES, OR
      $ 'F7.1' LBS. '/')
      1T31'SULPHUR LIQUID - 'F7.2' MOLES, OR 'F7.1' LBS. '/'
      1T32'(STREAM NO. 'I2' , TEMPERATURE = 'F6.1' DEG.F.))
2000  FORMAT(T34'SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,'
      $ /
      1T36'(LBS. S/100 LB. MOLES INERTS) = 'F6.2)
2001  FORMAT('0'T38'EXISTENCE OF COALESCER IS IMPLIED')
2002  FORMAT('0'T36'EXISTENCE OF DE-MISTER PADS IS IMPLIED')
2003  FORMAT('0'T44'REVISED SULPHUR OUTLET')
2004  FORMAT(' 'T36'-----')
3001  FORMAT(////T40'CONDENSER GASEOUS EXIT STREAM')
2010  FORMAT('0'T25'PERCENT CONDENSATION = 'F6.2',
      $ PERCENT RECOVERY =
      1'F6.2)
9000  FORMAT('0',T25,'*****')
      $*****
      1*****')
      END

```



```

C *****
C *
C *          SUBROUTINE COMBN
C *
C * FUNCTIONS -
C *
C * - PRIMARY ADIABATIC STREAM COMBINER ROUTINE
C * - DEFINES EQUIPMENT FEED
C * - CHECKS DATA FOR COMPATIBILITY
C * - FINDS ADIABATIC OUTLET TEMPERATURE
C *   (SULPHUR SHIFT REACTION ALLOWED ONLY)
C * - IF INFORMATION RECYCLE STREAM EXISTS, PREDICTS
C *   WHAT UPSTREAM STREAM SPLIT SHOULD BE TO YIELD
C *   DESIRED OUTLET TEMPERATURE. (USES RESULTS
C *   OF THIS PREDICTION AS PRESENT EQUIPMENT OUTLET
C *   STREAM)
C * - CALCULATES OUTLET STREAM SULPHUR AND WATER DEW
C *   POINTS AND STORES RESULTING OUTLET STREAM
C *
C *****

```

```

      SUBROUTINE COMBN
      COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
      COMMON /GEN2/TEMP, TFEED, YCOMP(20), YFEED(20), PRESS, ENTH
      COMMON /STOR1/EQUIP(300), ILOC, NMBEQ, STREM(50,22)
      $, NSIN(5), NSOUT(5)
      COMMON /BURN1/TCTOF, TBURN, IMUFF, NLGTH, NDIAM, NRTIM
      $, NHRLS, NBURN
      WRITE(IWRIT,6000) NMBEQ
      IF(ITEST-1) 803,802,802
802 WRITE(IWRIT,9000)
      WRITE(IWRIT,6001) NSIN(1),NSIN(2)
      WRITE(IWRIT,9000)
      WRITE(IWRIT,6003)
803 CONTINUE

```

```

C*****      DEFINE FEED STREAM.

```

```

      NSTRM=0
      CALL SUTIL(NSTRM,0,YFEED,TFEED,PRESS)

```

```

C*****      CHECK OUTLET TEMP. DATA FOR COMPATIBILITY.

```

```

      NEXIT=NSOUT(1)
      CALL COMPR(NEXIT,21,1)

```

```

C*****      FIND RESULTANT MIXED STREAM OUTLET TEMP.
C*****      SULPHUR SHIFT EQUILIBRIUM ALLOWED ONLY, SET TCTOF.

```

```

      TCTOF=-1.0
      DO 100 I=1,NTOT
100 YCOMP(I)=YFEED(I)

```


SUBROUTINE COMBN ... (CONT'D)

```

TEMP=TFEED
NOHLS=0
CALL TCALC(NOHLS)

```

```

C***** IF INFORMATION RECYCLE STREAM EXISTS, FIND THE
C***** STREAM SPLIT FRACTION, FOR FEED-BACK, WHICH WILL
C***** RESULT IN THE DESIRED OUTLET TEMP. FOR THIS
C***** EQUIPMENT.

```

```

      IF(NSOUT(2)) 200,300,300
200 CALL FINDE
300 CONTINUE

```

```

C***** DEFINE OUTLET STREAM.

```

```

      CALL SUTIL(NEXIT,2,YCOMP,TEMP,PRESS)
      EQUIP(ILOC+2)=TEMP
      IF(ITEST-1) 801,800,800
800 WRITE(IWRIT,9000)
      WRITE(IWRIT,6002)
      CALL PRNTS(NEXIT)

```

```

C***** CALCULATE OUTLET SULPHUR & WATER DEW PTS.

```

```

      TDEWS=500.
      CALL DEWPT(TDEWS,YCOMP,PRESS,1)
      TDEWW=150.
      CALL DEWPT(TDEWW,YCOMP,PRESS,0)
      WRITE(IWRIT,5002) TDEWS,TDEWW
      WRITE(IWRIT,9000)
801 CONTINUE
      RETURN
5002 FORMAT( ' T35' STREAM SULPHUR DEW PT. (DEG. F) = ',F7.1
      $/T35' STREAM W
      1LATER DEW PT. (DEG. F) = ',F7.1)
6000 FORMAT(T42' ADIABATIC STREAM COMBINER' /T45' EQUIPMENT
      $ NUMBER'
      1I3)
6001 FORMAT(T41,' COMBINE STREAMS ',I3,' AND 'I3)
6002 FORMAT(T32,' COMBINED OUTLET STREAM (SULPHUR SHIFT
      $ DONE) -')
6003 FORMAT(T32,' FIND GIVEN FEED STREAM RESULTANT
      $ TEMPERATURE')
9000 FORMAT('0',I25,' *****
      $*****
      1*****')
      END

```



```

C *****
C *
C *
C *          SUBROUTINE FINDE
C *
C *  FUNCTIONS -
C *
C *  -  STREAM SPLIT PREDICTOR ROUTINE
C *  -  DEFINES INFORMATION STREAM AND HOT AND COLD
C *      PROCESS INLET STREAMS
C *  -  USING THE SECANT METHOD, ITERATIVELY ESTIMATES
C *      UPSTREAM SPLIT TO YIELD DESIRED OUTLET
C *      TEMPERATURE
C *  -  FOR EACH ESTIMATE, EVALUATES EFFECTS ON HOT AND
C *      COLD STREAMS -- DOES SULPHUR SHIFT AND THEN
C *      FINDS RESULTING OUTLET TEMPERATURE (NEWTON'S
C *      METHOD)
C *  -  STORES PREDICTED SPLIT IN INFORMATION STREAM
C *      WHEN CONVERGENCE ACHIEVED
C *
C *****

```

```

      SUBROUTINE FINDE
      DIMENSION YFED1(20),YFED2(20)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFED(20),PRESS,ENTH
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)

```

```

C*****      DEFINE INFORMATION STREAM AND TWO FEED STREAMS.

```

```

      NINFO=-NSOUT(2)
      NEPSM=ABS(EQUIP(ILOC+3))+0.5
      NSTRM=NSIN(1)
      IF(NEPSM-NSTRM) 2,1,2
1  NSTRM=NSIN(2)
2  CALL SUTIL(NEPSM,1,YFED1,TEMP1,PDUMY)
      ENTH1=HFCAL(TEMP1,YFED1,0)
      CALL SUTIL(NSTRM,1,YFED2,TEMP2,PDUMY)
      ENTH2=HFCAL(TEMP2,YFED2,0)

```

```

C*****      DEFINE AND STORE PRESENT STREAM SPLIT FRACTION.

```

```

      EPS=SETVU(ABS(STREM(NINFO,2)),0.1)
      FPSTR=EPS

```

```

C*****      SET DESIRED OUTLET TEMP. AND ITERATION FLAGS.

```

```

      TDSIR=SETVU(-EQUIP(ILOC+1),425.0)
      FAC1=1.1
      FAC2=1.00
      TCALC=TEMP
      TEMP=TDSIR

```


SUBROUTINE FINDE ...(CONT'D)

```

KINIT=1
ITER=0
ERROR=TDSIR-TCALC
IF(ABS(ERROR/TDSIR)-CRIT*10.) 20,20,10

```

```

C***** CONVERGENCE CHECK.

```

```

9 IF(ABS(ERROR/TDSIR)-CRIT) 20,20,10

```

```

C***** SECANT METHOD IS USED TO GENERATE GUESSES FOR THE
C***** STREAM SPLIT FRACTION SUCH THAT THE DESIRED OUTLET
C***** TEMP. IS REALIZED.

```

```

10 CALL GUESR(EPS,FAC1,FAC2,ERROR,ITER)

```

```

C***** GENERATE NEW FEED STREAMS.

```

```

DO 11 I=1,NTOT
11 YCOMP(I)=YFED1(I)*EPS/EPSTR+YFED2(I)*(1-EPS)/(1-EPSTR)
    ENTHR=ENTH1*EPS/EPSTR+ENTH2*(1-EPS)/(1-EPSTR)

```

```

C***** CALCULATE SULPHUR SHIFT AT DESIRED TEMP. (TDSIR)

```

```

CALL SHIFT(KINIT,NTOT)

```

```

C***** CALCULATE RESULTING OUTLET STREAM TEMP.

```

```

CALL FINDT(YCOMP,TCALC,ENTHR)
ERROR=TDSIR-TCALC
IF(ITEST-5) 801,800,800
800 WRITE(IWRIT,5000) ITER,TDSIR,TCALC,EPS,EPSTR
801 GO TO 9
20 CONTINUE

```

```

C***** STORE FOUND STREAM SPLIT FRACTION.

```

```

STREAM(NINFO,2)=EPS
IF(ITEST-1) 803,802,802
802 WRITE(IWRIT,9000)
    WRITE(IWRIT,5001) TDSIR,EPS
    WRITE(IWRIT,5002)
803 CONTINUE
    RETURN
5000 FORMAT(' 'FINDE' ' ITER = ',I3,' TDSIR = 'F10.4,'
$ TCALC = ',F10.4,
1' EPS = ',F10.4,' EPSTR = ',F10.4)
5001 FORMAT(T26'PREDICTED STREAM SPLIT FOR TEMP. OF 'F10.4
$, ' IS 'F7.4)
5002 FORMAT(T34'USE STREAMS RESULTING FROM THIS PREDICTION
$ '/')

```


SUBROUTINE FINDE ... (CONT'D)

```
1T36 'FOR PRESENT EQUIPMENT OUTLET STREAM.')
```

9000 FORMAT('O',T25,'*****')

\$*****

1*****')

END


```

C *****
C *
C *          SUBROUTINE CMBDV
C *
C *  FUNCTIONS -
C *
C *  -  PRIMARY STREAM COMBINER/DIVIDER ROUTINE
C *  -  COMBINES UP TO 5 INLET STREAMS AND CALCULATES
C *      RESULTING TEMPERATURE AND PRESSURE
C *  -  DIRECTS COMBINED STREAMS TO A SINGLE OUTPUT
C *      OR DIVIDES THE STREAM BETWEEN TWO OUTLETS
C *
C *****

```

```

      SUBROUTINE CMBDV
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
      COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
      $,NSIN(5),NSOUT(5)
      DATA IAND/'&'/
      WRITE(IWRIT,6000) NMBEQ

```

```

C*****      CHECK NUMBER OF INLET AND OUTLET STREAMS.

```

```

      DO 1 I=1,5
      IF(NSIN(I)) 2,2,1
1 CONTINUE
2 KIN=I-1
      DO 3 I=1,5
      IF(NSOUT(I)) 4,4,3
3 CONTINUE
4 KOUT=I-1

```

```

C*****      DEFINE TOTAL FEED TO EQUIP.

```

```

      NSTRM=0
      CALL SUTIL(NSTRM,0,YFEED,TFEED,PRESS)

```

```

C*****      KIN=1, SINGLE FEED.  KIN G.T. 1, COMBINER.

```

```

      IF(KIN-1) 11,11,10
10 IF(ITEST-1) 801,800,800
800 WRITE(IWRIT,9000)
      WRITE(IWRIT,1000) NSIN(1),(IAND,NSIN(I),I=2,KIN)
11 CALL PRNTS(-1)
801 CONTINUE

```

```

C*****      KOUT=1, SINGLE OUTLET.  KOUT=2, DIVIDER.

```

```

      IF(KOUT-2) 20,21,500

```

```

C*****      STORE SINGLE OUTLET.

```


SUBROUTINE CMBDV ...{CONT'D}

```

20 CALL SUTIL(NSOUT(1),2,YFEED,TFEED,PRESS)
   GO TO 900
500 WRITE(IWRIT,5000)
21 EPS=SETVU(ABS(EQUIP(ILOC+1)),0.1)
   EQUIP(ILOC+1)=SIGN(EPS,EQUIP(ILOC+1))
   NSPLT=ABS(EQUIP(ILOC+2)) +0.5
   NEXIT=NSOUT(1)
   IF(NEXIT-NSPLT) 22,23,22
23 NEXIT=NSOUT(2)
22 CONTINUE
   THRU=1.0-EPS
   DO 30 I=1,NTOT
   YCOMP(I)=YFEED(I)*EPS
   YFEED(I)=YFEED(I)*THRU
30 CONTINUE

C*****   STORE SPLIT AND THROUGH STREAMS.

   CALL SUTIL(NEXIT,2,YFEED,TFEED,PRESS)
   CALL SUTIL(NSPLT,2,YCOMP,TFEED,PRESS)
   IF(ITEST-1) 803,802,802
802 THRU=THRU*100.0
   EPS=EPS*100.0
   WRITE(IWRIT,1002) EPS,NSPLT,THRU,NEXIT
   WRITE(IWRIT,9000)
803 CONTINUE
900 RETURN
1000 FORMAT('0'T39,'COMBINE STREAMS 'I2,4(' 'A1' 'I2))
1002 FORMAT('0'T45'TOTAL FEED IS SPLIT -'//T41,F7.3'
   $ PERCENT TO STREAM
   1'I4' ,'/T41,F7.3,' PERCENT TO STREAM'I4)
5000 FORMAT('0A STREAM DIVIDER HAS 2 OUTLET STREAMS, NO
   $ MORE')
6000 FORMAT(T43'STREAM COMBINER / DIVIDER'/T45
   1'EQUIPMENT NUMBER 'I3)
9000 FORMAT('0',T25,'*****')
   $*****
   1*****')
END

```



```

C *****
C *
C *
C *
C * FUNCTIONS -
C *
C * - PRIMARY COMBUSTION AIR ADDER ROUTINE
C * - DEFINES ACID GAS FEED AND IDENTIFIES AIR STREAM
C * - FINDS AIR REQUIREMENTS AND ADDS AIR TO ACID
C *   GAS TO FORM OUTPUT STREAM
C * - STORES OUTPUT AND AIR INLET STREAMS
C *
C *****

```

```

SUBROUTINE AIRAD
  DIMENSION YAIP(20)
  COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
  COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
  COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
  $,NSIN(5),NSOUT(5)
  COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)
  WRITE(IWRIT,6000) NMBEQ
  NAIR=ABS(EQUIP(ILOC+1))+0.5
  NSTRM=NAIR
  CALL SUTIL(NSTRM,0,YFEED,TFEED,PRESS)
  CALL PRNITS(-1)
  CALL COMPR(NAIR,21,3)
  CALL COMPR(NAIR,22,4)
  RELHY=SETVU(-EQUIP(ILOC+2),50.0)
  TAIR=SETVU(-EQUIP(ILOC+3),70.0)
  PAIR=SETVU(-EQUIP(ILOC+4),PRESS)
  SPEC1=SETVU(-EQUIP(ILOC+5),1.0)
  SPEC2=SETVU(-EQUIP(ILOC+6),1.0)
  DO 1 I=1,NTOT
1  YCOMP(I)=YFEED(I)
  TEMP=TFEED
  CALL AIRFD(YCOMP,TEMP,SPEC1,SPEC2,RELHY,YAIR,TAIR
  $,PAIR)
  EQUIP(ILOC+2)=SIGN(RELHY,EQUIP(ILOC+2))
  EQUIP(ILOC+3)=SIGN(TAIR,EQUIP(ILOC+3))
  EQUIP(ILOC+4)=SIGN(PAIR,EQUIP(ILOC+4))
  EQUIP(ILOC+5)=SIGN(SPEC1,EQUIP(ILOC+5))
  EQUIP(ILOC+6)=SIGN(SPEC2,EQUIP(ILOC+6))
  PRESS=AMIN1(PRESS,PAIR)
  NEXIT=NSOUT(1)
  CALL SUTIL(NEXIT,2,YCOMP,TEMP,PRESS)
  CALL SUTIL(NAIR,2,YAIR,TAIR,PAIR)
  IF(ITEST-1) 801,800,800
800 TOT=0.0
  DO 2 I=1,NTOT
2  TOT=TOT+YAIR(I)
  TOTDA=TOT-YAIR(IDH2O)

```


SUBROUTINE AIRAD ... (CONT'D)

```

      WRITE(IWRIT,1000)TOT,RELHY,TOTDA,YAIR(IDH2O),TAIR,PAIR
      $,SPEC2,SPEC1
      WRITE(IWRIT,9000)
      WRITE(IWRIT,1001)
      CALL PRNTS(NEXIT)
801  CONTINUE
      RETURN
1000  FORMAT(T25'TOTAL MOLES AIR ADDED = 'F8.2,T62'(R.H. =
      $ 'F6.2' PERCENT
      1T)'/T25'MOLES DRY AIR = 'F8.2,T63'MOLES WATER = 'F8.2
      $/T25'TEMPERAT
      1URE (DEG.F.) = 'F6.1,T60'PRESSURE (PSIA.) = 'F6.2/
      $/T31'RATIO OF (S
      1PECIFIED/STOICHIOMETRIC) AIR ADDED -'/T27'- FOR
      $ OXIDATION OF SULP
      1HUR (ALL H2S) -'T76,F7.4/T27'- FOR OXIDATION OF
      $ CARBON, HYDROGEN
      1AND ABOVE -'T76,F7.4)
1001  FORMAT(T44'COMBINED OUTLET STREAM')
6000  FORMAT(T45,'COMBUSTION AIR ADDER'/T45'EQUIPMENT NUMBER
      $ ',I3)
9000  FORMAT('0',T25,'*****')
      $*****
      1*****')
      END

```



```

C *****
C *
C *          SUBROUTINE INCIN
C *
C *  FUNCTIONS -
C *
C *  - PRIMARY TAIL GAS INCINERATOR ROUTINE
C *  - IDENTIFIES FUEL GAS STREAM AND DEFINES FEED
C *  - VAPORIZES ANY INLET LIQUID SULPHUR
C *  - SIMULATION -- COMBINES PROCESS GAS INLET AND
C *    (FUEL AND AIR) INLET AND DETERMINES THE
C *    ADIABATIC FLAME TEMPERATURE
C *  - DESIGN -- ITERATIVELY ESTIMATES THE AMOUNT OF
C *    FUEL (AND AIR) REQUIRED TO ACHIEVE THE DESIRED
C *    OUTLET TEMPERATURE. FOR EACH ESTIMATED FUEL AND
C *    AIR ADDITION, CALCULATES RESULTING TEMP.
C *  - CONVERGENCE ACHIEVED USING SECANT METHOD
C *  - STORES OUTLET STREAM (AND AIR AND FUEL STREAM
C *    FOR THE DESIGN CASE)
C *
C *****

```

```

SUBROUTINE INCIN.
  DIMENSION YAIR(20),YGAS(20)
  COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
  COMMON /GEN2/TEMP,TFEED,YCOMP(20),YFEED(20),PRESS,ENTH
  COMMON /STOR1/EQUIP(300),ILOC,NMBEQ,STREM(50,22)
  $,NSIN(5),NSOUT(5)
  COMMON /DATA5/IDH2O,IDSUL(5),WTMOL(20),VMOLE(20)
  WRITE(IWRIT,6000) NMBEQ
  NGAS=ABS(EQUIP(ILOC+7))+0.5
  CALL SUTIL(NGAS,1,YGAS,TGAS,PGAS)
  NSTRM=NGAS
  CALL SUTIL(NSTRM,0,YFEED,TFEED,PRESS)
  CALL PRNTS(-1)
  ENTHR=HFCAL(TFEED,YFEED,0)
  ISUL=IDSUL(1)
  DO 1 I=1,5
    IF(IDSUL(I)-NGMS) 1,1,2
  2 ILIQ=IDSUL(I)
    YFEED(ISUL)=YFEED(ISUL)+YFEED(ILIQ)*WTMOL(ILIQ)
    $/WTMOL(ISUL)
    YFEED(ILIQ)=0
  1 CONTINUE
  CALL FINDT(YFEED,TFEED,ENTHR)
  CALL COMPR(NSOUT(1),21,1)
  TDSIR=-EQUIP(ILOC+1)
  IF(TDSIR) 11,11,13
  11 ISIM=1
    IF(ITEST-2) 801,800,800
  800 WRITE(IWRIT,1000)
    CALL PRNTS(NGAS)

```


SUBROUTINE INCIN ... (CONT'D)

```

801 CONTINUE
   NOHLS=0
   TEMP=1200.
   DO 12 I=1,NTOT
     YCOMP(I)=YFEED(I)+YGAS(I)
12  YFEED(I)=YCOMP(I)
     ENTHR=ENTHR+HFCAL(TGAS,YGAS,0)
     CALL FINDT(YFEED,TFEED,ENTHR)
     CALL TCALC(NOHLS)
     IF(ITEST-1) 807,806,806
806 WRITE(IWRIT,9000)
807 CONTINUE
     GO TO 500
13  ISIM=0
     RELHY=SETVU(-EQUIP(ILOC+2),50.)
     TAIR=SETVU(-EQUIP(ILOC+3),70.)
     PAIR=SETVU(-EQUIP(ILOC+4),PRESS)
     SPEC1=SETVU(-EQUIP(ILOC+5),1.25)
     SPEC2=SETVU(-EQUIP(ILOC+6),1.25)
     CALL AIRFD(YGAS,TGAS,SPEC2,1.0,RELHY,YAIR,TAIR,PAIR)
     ENTH2=HFCAL(TGAS,YGAS,0)
     CALL AIRFD(YFEED,TFEED,SPEC1,1.0,RELHY,YAIR,TAIR,PAIR)
     ENTH1=HFCAL(TFEED,YFEED,0)
     FAC1=2.0
     FAC2=1.0
     ITERH=0
     KINIT=1
     FACTR=1.0
100 CALL GUESR(FACTR,FAC1,FAC2,ERROR,ITERH)
     DO 31 I=1,NTOT
31  YCOMP(I)=YFEED(I)+YGAS(I)*FACTR
     ENTHR=ENTH1+ENTH2*FACTR
     CALL MINFE(PRESS,TDSIR,YCOMP,KINIT)
     ENTHN=HFCAL(TDSIR,YCOMP,0)
     ERROR=ENTHN-ENTHR
     IF(ITEST-3) 805,804,804
804 WRITE(IWRIT,2000) ITERH,FACTR,ENTHR,ENTHN
805 CONTINUE
     IF(ABS(ERROR/ENTHR)-CRIT) 40,40,100
40  TEMP=TDSIR
     ENTHR=HFCAL(TAIR,YAIR,0)+ENTH2*FACTR
     DO 41 I=1,NTOT
41  YGAS(I)=YGAS(I)*FACTR+YAIR(I)
     CALL FINDT(YGAS,TGAS,ENTHR)
     CALL SUTIL(NGAS,2,YGAS,TGAS,PGAS)
     EQUIP(ILOC+2)=SIGN(RELHY,EQUIP(ILOC+2))
     EQUIP(ILOC+3)=SIGN(TAIR,EQUIP(ILOC+3))
     EQUIP(ILOC+4)=SIGN(PAIR,EQUIP(ILOC+4))
     EQUIP(ILOC+5)=SIGN(SPEC1,EQUIP(ILOC+5))
     EQUIP(ILOC+6)=SIGN(SPEC2,EQUIP(ILOC+6))

```


SUBROUTINE INCIN ... (CONT'D)

```

      IF(I TEST-1) 803,802,802
802  WRITE(IWRIT,1001) TAIR,PAIR,RELHY,SPEC1,SPEC2
      WRITE(IWRIT,9000)
      WRITE(IWRIT,1000)
803  CONTINUE
      CALL PRNTS(NGAS)
500  CONTINUE
      NEXIT=NSOUT(1)
      CALL SUTIL(NEXIT,2,YCOMP,TEMP,PRESS)
      IF(I TEST-1) 811,810,810
810  WRITE(IWRIT,9001)
      CALL PRNTS(NEXIT)
811  CONTINUE
      RETURN
1000 FORMAT(T45'FUEL AND AIR STREAM')
1001 FORMAT(T25'COMBUSTION AIR -'/T30'TEMPERATURE(DEG.F) ='
$ ,T74,F7.1/
      1T30'PRESSURE (PSIA.) ='T74,F7.2/T30'RELATIVE HUMIDITY
$ (PERCENT) ='
      1T74,F7.2//T25'RATIO (SPECIFIED/STOICHIOMETRIC) AIR
$ ADDED -'/
      1T30'FOR COMBUSTION OF PROCESS GAS -'T74,F7.3/T30'FOR
$ COMBUSTION OF
      1 FUEL GAS -'T74,F7.3)
2000 FORMAT(' ITERH ='I3'  FACTR='F10.4'  ENTHR='E15.7'
$ ENTHN ='F15.7)
6000 FORMAT(T43'EXHAUST GAS INCINERATOR'/T45
      1 'EQUIPMENT NUMBER 'I3)
9001 FORMAT('1'////T42'INCINERATOR EXHAUST STREAM')
9000 FORMAT('0',T25,'*****')
      1*****
      1*****')
      END

```



```

C *****
C *
C * SUBROUTINE STACK *
C *
C * FUNCTIONS - *
C *
C * - PRIMARY EXHAUST GAS STACK ROUTINE *
C * - IDENTIFIES SO2 (POLLUTANT SPECIE) *
C * - CALCULATES EQUIVALENT AMBIENT AND STACK OUTLET *
C * TEMPERATURES, TOTAL AND POLLUTANT FLOWRATES *
C * AND STACK VELOCITY *
C * - DETERMINES REQUIRED STACK HEIGHT (DESIGN) OR *
C * MAX GROUND CONCENTRATION OF POLLUTANT *
C * (SIMULATION) *
C * - OPTIONALLY DESIGNS SEVERAL STACKS WITH VARYING *
C * STACK VELOCITIES *
C *
C *****

```

```

SUBROUTINE STACK
COMMON /GEN1/IWRIT, IDBUG(15), ITEST, CRIT, NGMS, NTOT
COMMON /GEN2/TEMP, TFEED, YCOMP(20), YFEED(20), PRESS, ENTH
COMMON /STOR1/EQUIP(300), ILOC, NMBEQ, STREM(50,22)
$, NSIN(5), NSOUT(5)
COMMON /DATA1/FORMU(20,5), NATYP, IDATM(5)
COMMON /DATA5/IDH2O, IDSUL(5), WTMOL(20), VMOLF(20)
COMMON /STAK1/ISIM, QTOT, VSTAK, TSTAK, TEQIV, QSO2
COMMON /STAK2/CMAX(2), HSTAK(2), EMAX(2), DMAX(2), VMAX(2)
WRITE(IWRIT,6000) NMBEQ
NSTRM=0
CALL SUTIL(NSTRM,0,YFEED,TFEED,PRESS)
CALL PRNTS(-1)
NEXIT=IABS(NSOUT(1))

```

```

C***** IDENTIFY SO2 SPECIE.

```

```

DO 1 I=1,NGMS
IF(ABS(WTMOL(I)-64.)-0.1) 2,1,1
2 IDS=IDATM(1)
IF(ABS(FORMU(I,IDS)-1.)-0.1) 3,1,1
3 IDO=IDATM(2)
IF(ABS(FORMU(I,IDO)-2.)-0.1) 4,1,1
4 ISO2=I
GO TO 5
1 CONTINUE
WRITE(IWRIT,5000)

```

```

C***** CALCULATE EQUIVALENT AMBIENT TEMP. AND AMBIENT
C***** TOTAL AND SO2 FLOW RATES (CU.FT./SEC.).

```

```

5 CALL SUMER(YFEED,NGMS,0,YTOT,TMASS)
TAMBI=SETVJ(-EQUIP(ILOC+1),70.)

```


SUBROUTINE STACK ... (CONT'D)

```

TEQIV=TMASS/YTOT/29.*TAMBI
FACTR=10.73*(TEQIV+460.)/(PRESS*3600.)
QTOT=YTOT*FACTR
QSO2=YFEED(ISO2)*FACTR
TSTAK=SETVU(-EQUIP(ILOC+2),TFEED-200.)
CALL SUTIL(NEXIT,2,YFEED,TSTAK,PRESS)
DO 6 I=1,2
  CMAX(I)=0.0
6  HSTAK(I)=0.0
  ICNT=1
  HIGH=-EQUIP(ILOC+3)
  IF(HIGH) 20,20,10
10  DIAM=-EQUIP(ILOC+4)
  IF(DIAM) 20,20,11
11  ISIM=1
  HSTAK(1)=HIGH
  HSTAK(2)=HIGH
  NDO=1
  VSTAK=4.*QTOT/(3.14159*DIAM**2)
  GO TO 25
20  ISIM=0
  NDO=SETVU(-EQUIP(ILOC+8),1.)+0.5
  VSTAK=SETVU(-EQUIP(ILOC+6),60.)
  DELSK=SETVU(-EQUIP(ILOC+7),20.)
  CMAX(1)=SETVU(-EQUIP(ILOC+5),0.20)
  CMAX(2)=CMAX(1)
25  IF(ITEST-1) 801,800,800
800  IF(ISIM) 804,804,805
804  WRITE(IWRIT,1050)
  GO TO 806
805  WRITE(IWRIT,1051)
806  WRITE(IWRIT,1000) TAMBI,TEQIV,QTOT,QSO2,TSTAK
  WRITE(IWRIT,9000)
801  CONTINUE
  IF(ISIM) 29,29,30
29  DIAM=(4.*QTOT/(3.14159*VSTAK))**0.5
30  CALL STAKU
  IF(ITEST-1) 803,802,802
802  WRITE(IWRIT,1001) DIAM,VSTAK
  WRITE(IWRIT,1002)
  WRITE(IWRIT,1003) HSTAK(1),HSTAK(2),CMAX(1),CMAX(2)
  $,VMAX(1),
  1 VMAX(2),DMAX(1),DMAX(2),EMAX(1),FMAX(2)
  WRITE(IWRIT,9000)
803  CONTINUE
  IF(ICNT-NDO) 31,32,32
31  ICNT=ICNT+1
  VSTAK=VSTAK+DELSK
  GO TO 20
32  CONTINUE

```


SUBROUTINE STACK ... (CONT'D)

```

EQUIP(ILOC+1)=SIGN(TAMBI,EQUIP(ILOC+1))
EQUIP(ILOC+2)=SIGN(TSTAK,EQUIP(ILOC+2))
HIGH=AMAX1(HSTAK(1),HSTAK(2))
EQUIP(ILOC+3)=SIGN(HIGH,EQUIP(ILOC+3))
EQUIP(ILOC+4)=SIGN(DIAM,EQUIP(ILOC+4))
PPM=AMAX1(CMAX(1),CMAX(2))
EQUIP(ILOC+5)=SIGN(PPM,EQUIP(ILOC+5))
EQUIP(ILOC+6)=SIGN(VSTAK,EQUIP(ILOC+6))
EQUIP(ILOC+7)=SIGN(DELSK,EQUIP(ILOC+7))
RDO=NDO
EQUIP(ILOC+8)=SIGN(RDO,EQUIP(ILOC+8))
RETURN
1000 FORMAT(/T25'AMBIENT TEMPERATURE (DEG.F) ='T78,F7.1
$/T25'EQUIVALENT
1 STACK TEMPERATURE (DEG.F) ='T78,F7.1/T25'TOTAL
$ GASEOUS STACK FLOW
1RATE (C.F.S. AT TEQIV) ='T78,F7.1/T25'POLLUTANT (SO2)
$ FLOWRATE (C.
1F.S. AT TEQIV) ='T78,F7.3/T25'STACK OUTLET TEMPERATURE
$ (DEG.F) ='T
178,F7.1)
1001 FORMAT('0'T25'STACK DIAMETER (FT. AT TOP) ='T78,F7.2
$/T25'STACK VEL
1OCITY (FT/SEC. AT TOP) ='T78,F7.2)
1002 FORMAT(/T63'ATMOSPHERIC CONDITIONS'/T63'-----
$-----
1/T63' STABLE UNSTABLE'/T63'-----
$-'/)
1003 FORMAT(T25'STACK HEIGHT (FT.) ='T59,2F12.1/T25 'MAX.
$ GROUND CONC
1ENTRATION (PPM) ='T59,2F12.4/T25'WIND SPEED AT MAX.
$ (FT/SEC) ='
1T59,2F12.2/T25'DISTANCE (SOURCE TO MAX., FT.) ='T59
$,2F12.0/T25
1'EFFECTIVE STACK HEIGHT (FT.) ='T59,2F12.1)
1050 FORMAT(T25'SULPHUR PLANT STACK',T79'DESIGN')
1051 FORMAT(T25'SULPHUR PLANT STACK'T75'SIMULATION')
5000 FORMAT('0 ERROR W.R.T. PRESENCE OF SO2 SPECIE.')
6000 FORMAT(T45'SULPHUR PLANT STACK'/T45'EQUIPMENT
$ NUMBER'I3)
9000 FORMAT('0',T25,'*****')
$*****
1*****'/)
END

```



```

C *****
C *
C *          SUBROUTINE STAKU
C *
C *  FUNCTIONS -
C *
C *  -  STACK UTILITY ROUTINE
C *  -  CALCULATES MAXIMUM GROUND CONCENTRATION OF
C *      POLLUTANT (SO2) AND DISTANCE TO THE MAXIMUM AT
C *      SEVERAL WIND VELOCITIES FOR BOTH MODERATELY
C *      STABLE AND MODERATELY UNSTABLE ATMOSPHERIC
C *      CONDITIONS
C *  -  THE MINIMUM STACK HEIGHT REQUIRED FOR A
C *      MAXIMUM ALLOWABLE GROUND CONCENTRATION
C *      IS FOUND IN THE DESIGN CASE.
C *  -  FOR THE SIMULATION CASE, THE MAXIMUM GROUND
C *      CONCENTRATION, THE CORRESPONDING WIND SPEED
C *      AND DISTANCE TO THE MAXIMUM FOR A GIVEN STACK
C *      HEIGHT ARE FOUND
C *
C *****

```

```

      SUBROUTINE STAKU
      REAL J
      DIMENSION WVFL(10),AMU(10),GFACT(10),TITLE(2,2)
      COMMON /GEN1/IWRIT,IDBUG(15),ITEST,CRIT,NGMS,NTOT
      COMMON /STAK1/ISIM,QTOT,VSTAK,TSTAK,TEQIV,QSO2
      COMMON /STAK2/CMAX(2),HSTAK(2),EMAX(2),DMAX(2),VMAX(2)
      DATA WVFL/1.,5.,7.34,10.,14.67,20.,22.,29.34,36.67,44.
      $/
      DATA AMU/.5,.1,.068,.056,.034,.016,.0114,.0051,.0041
      $,.0034/
      DATA GFACT/.7292,.7292,.7292,.7905,.8930,.9904,1.0295,
      1 1.7862,2.3964,3.1057/
      DATA TITLE/' STA','BLE ','UNST','ABLE'/
      TFCN(Z,WINDV)=6.37*32.17*QTOT*DELT*Z/(TRANK*WINDV**3)
      DELT=TSTAK-TEQIV
      TRANK=TEQIV+460.
      SQQV=SQRT(QTOT*VSTAK)
      VELMN=SQRT(32.17*DELT/TRANK*SQRT(QTOT/VSTAK))
      DO 500 I=2,10
      SQR=GFACT(I)*SQRT(TRANK)
      VRISE=4.77/(1.+0.43*WVFL(I)/VSTAK)*SQQV/WVFL(I)
      PROD=2.35E5*QSO2*AMU(I)
      DO 400 K=1,2
      IF(K-1) 50,50,51
50  J=WVFL(I)**2/SQQV*(SQR-0.28*VSTAK*TRANK/(32.17*DELT))
      $+1.0
      Z=ALOG(J**2)+2./J-2.
      GO TO 70
51  XA=DISTX
61  XB=XA*WVFL(I)/(3.57*SQQV)

```


SUBROUTINE STAKU ... (CONT'D)

```

        IF(XB-20.0) 62,63,63
62     Z=XB/(2.172+0.1359*XB)
        GO TO 64
63     Z=(ALOG(XB)/2.303-0.3553)/0.2286
64     IF(ISIM) 70,70,65
65     TRISE=TFCN(Z,WVEL(I))
        ESH=0.75*(VRISE+TRISE)+HSTAK(K)
        DIST=10.0*ESH
        TH=DIST-XA
        IF(ABS(TH)-XA/1000.) 73,73,66
66     XA=XA+TH/2.
        GO TO 61
70     TRISE=TFCN(Z,WVEL(I))
        IF(ISIM) 71,71,72
71     ESH=(PROD/CMAX(K))**0.5
        CTEMP=CMAX(K)
        DIST=ESH*10.*(3-K)
        DISTX=ESH*10.0
        HTEMP=ESH-(VRISE+TRISE)*0.75
        IF(HTEMP-HSTAK(K)) 300,300,100
100    HSTAK(K)=HTEMP
        GO TO 201
72     ESH= (TRISE+VRISE)*0.75+HSTAK(K)
        DISTX=ESH*20.0
73     CTEMP=PROD/ESH**2
        DIST=ESH*10.*(3-K)
        HTEMP=HSTAK(K)
        IF(CTEMP-CMAX(K)) 300,300,200
200    CMAX(K)=CTEMP
201    VMAX(K)=WVEL(I)
        DMAX(K)=DIST
        EMAX(K)=ESH
200    IF(ITEST-3) 801,800,800
800    WRITE(IWRIT,1000) (TITLE(KK,K),KK=1,2),WVEL(I),TRISE
        1,VRISE,ESH,DIST,CTEMP,HTEMP
801    CONTINUE
        IF(WVEL(I)-VELMN) 500,400,400
400    CONTINUE
500    CONTINUE
        RETURN
1000   FORMAT('0',T25,2A4,T70,'WVEL = 'F7.2/T25'TRISE = 'F9.0
        $,4X,'VRISE =
        1 'F9.0,4X,' ESH = 'F9.0/T25' DIST = 'F9.0,4X,'CTEMP =
        $ 'F9.3,4X,'H
        1TEMP = 'F9.0)
        END

```


APPENDIX E

EXAMPLES OF PROGRAM USE

EXAMPLE 1. E-2

EXAMPLE 2. E-53

EXAMPLE 3. E-89

EXAMPLE 4. E-125

EXAMPLE 5. E-142

EXAMPLE 1.

SPECIFICATIONS

PLANT FEED	ACID GAS, MOLES/HR.
CH4	1.5677
CO2	104.2917
H2O	47.0
H2S	290.0417

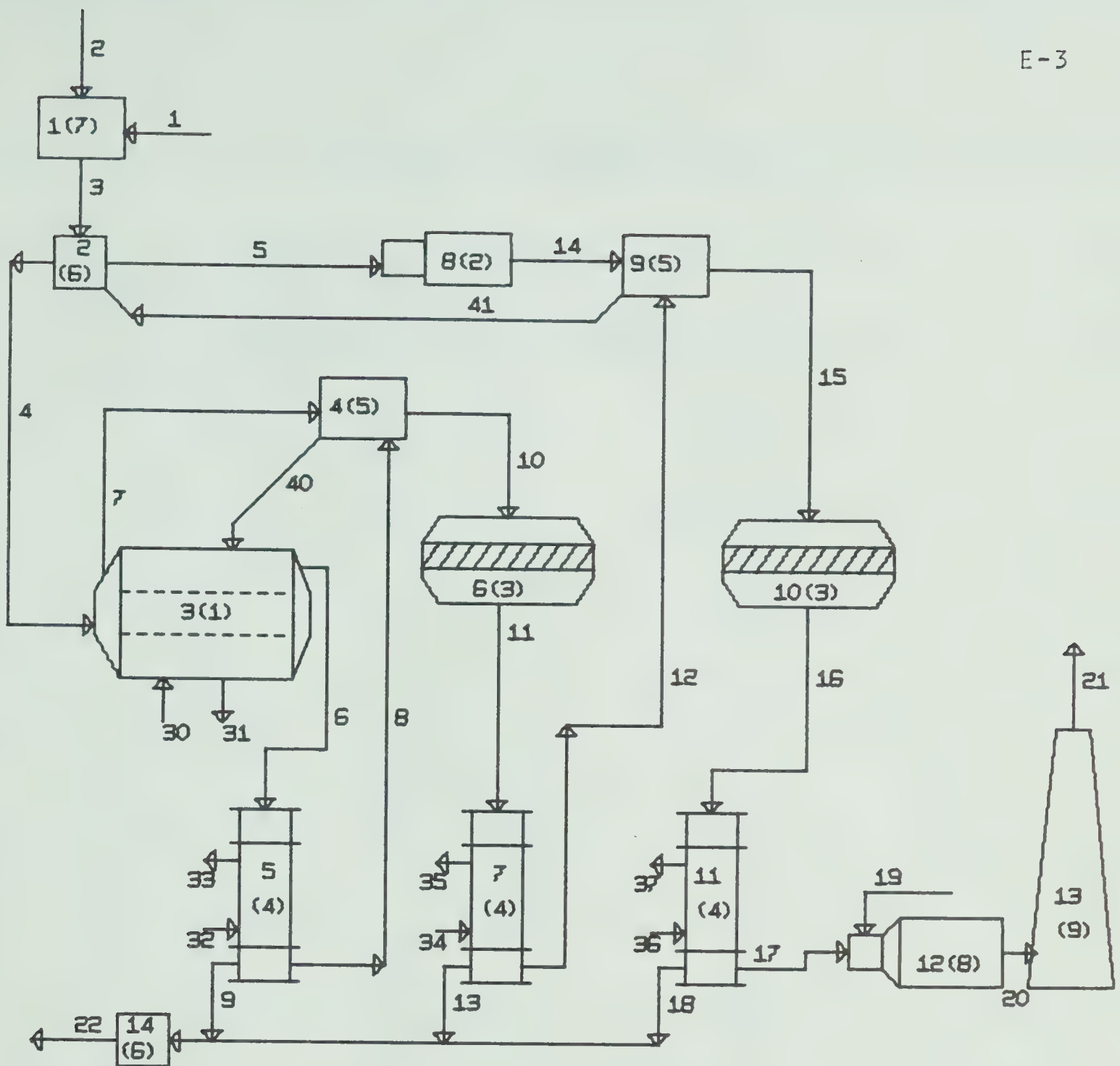
COMBUSTION AIR	PERCENT OF STOICHIOMETRIC REQUIREMENTS
100	100
105	105
110	110
115	115
120	120
125	125
130	130
135	135
140	140
145	145
150	150
155	155
160	160
165	165
170	170
175	175
180	180
185	185
190	190
195	195
200	200
205	205
210	210
215	215
220	220
225	225
230	230
235	235
240	240
245	245
250	250
255	255
260	260
265	265
270	270
275	275
280	280
285	285
290	290
295	295
300	300
305	305
310	310
315	315
320	320
325	325
330	330
335	335
340	340
345	345
350	350
355	355
360	360
365	365
370	370
375	375
380	380
385	385
390	390
395	395
400	400
405	405
410	410
415	415
420	420
425	425
430	430
435	435
440	440
445	445
450	450
455	455
460	460
465	465
470	470
475	475
480	480
485	485
490	490
495	495
500	500
505	505
510	510
515	515
520	520
525	525
530	530
535	535
540	540
545	545
550	550
555	555
560	560
565	565
570	570
575	575
580	580
585	585
590	590
595	595
600	600
605	605
610	610
615	615
620	620
625	625
630	630
635	635
640	640
645	645
650	650
655	655
660	660
665	665
670	670
675	675
680	680
685	685
690	690
695	695
700	700
705	705
710	710
715	715
720	720
725	725
730	730
735	735
740	740
745	745
750	750
755	755
760	760
765	765
770	770
775	775
780	780
785	785
790	790
795	795
800	800
805	805
810	810
815	815
820	820
825	825
830	830
835	835
840	840
845	845
850	850
855	855
860	860
865	865
870	870
875	875
880	880
885	885
890	890
895	895
900	900
905	905</

HYDROCARBON FEED	100.
HYDROGEN SULPHIDE FEED	33.3
PROCESS GAS TO INCINERATOR	125.
FUEL GAS TO INCINERATOR	100.

SPECIFIED TEMPERATURES AND PRESSURES	DEG.F.	PSIA.
AMBIENT	75.	
ACID GAS FEED	70.	19.
PRIMARY COMBUSTION AIR (R.H. = 45)	75.	18.5
INCINERATOR FUEL GAS (METHANE)	100.	13.
INCINERATOR COMBUSTION AIR (R.H. = 55)	80.	15.
BOILER BYPASS	900.	
BOILER EXIT	600.	
PRIMARY (BOILER) EQUILIBRIUM CUTOFF	1600.	
NO. 1. CONVERTER INLET	450.	
NO. 2. CONVERTER INLET	425.	
INCINERATOR PROCESS EXIT	1250.	
STACK EXIT	1175.	

MISCELLANEOUS

- 3 PASS BOILER WITH FIRST PASS FIRE-TUNNEL
- MAXIMUM ALLOWABLE PRESSURE DROPS IN 2ND AND 3RD BOILER PASSES 0.6 AND 0.9 PSIA RESPECTIVELY.
- MIN. FLAME REACTION RESIDENCE TIME 0.6 SEC.
- AVERAGE CATALYST PARTICLE SIZE 0.15 IN.
- MAXIMUM ALLOWABLE FOG IN 1ST, 2ND, AND 3RD CONDENSERS 25, 13, AND 4 LB.(S)/100 MOLES INERT EXIT GAS RESPECTIVELY
- MAX. HEAT RELEASE FOR INLINE BURNER 50,000 BTU/HR.CU.FT.
- MAXIMUM GROUND LEVEL CONCENTRATION OF SO₂ 0.2 PPM
- STACK EXIT VELOCITY 80 FT/SEC.



LEGEND

NUMBERS DENOTE STREAM OR EQUIPMENT NUMBERS

NUMBERS IN BRACKETS DENOTE EQUIPMENT TYPES -

- | | |
|------------------------|---------------------|
| 1. WASTE HEAT BOILER | 6. COMBINER/DIVIDER |
| 2. INLINE BURNER | 7. AIR ADDER |
| 3. CATALYTIC CONVERTER | 8. INCINERATOR |
| 4. SULPHUR CONDENSER | 9. EFFLUENT STACK |
| 5. ADIABATIC COMBINER | 10. BLACK BOX |

FIG. E-1 EQUIPMENT MODULE (PROCESS)
FLOWSHEET FOR EXAMPLE 1.

PROGRAM DATA (CARD IMAGE)

C EXAMPLE 1. (DESIGN)

PROGRAM CONTROL PARAMETERS

1 1 1 1 1 1 1 1 1 1 0 0 0 5 1

' PRINT SUPPRESS ' *END*

FLOWSHEET DATA

1	0	1			**
2	0	1			**
3	1	2			**
4	2	3			**
5	2	3			**
6	3	5			**
7	3	4			**
8	5	4			**
9	5	14			**
10	4	6			**
11	6	7			**
12	7	9			**
13	7	14			**
14	8	9			**
15	9	10			**
16	10	11			**
17	11	12			**
18	11	14			**
19	0	12			**
20	12	13			**
21	13	0			**
22	14	0			**
30	0	3	0	1	**
31	3	0	0	1	**
32	0	5	0	1	**
33	5	0	0	1	**
34	0	7	0	1	**
35	7	0	0	1	**
36	0	11	0	1	**
37	11	0	0	1	**
40	4	3	1	-1	**
41	9	2	1	-1	**

END

STREAM SPECIFICATIONS

1 1 1.5677 2 104.2917 5 47. 6 290.0417 21 70. 22 19. **
 19 1 20.91 21 100. 22 13. **
 40 1 19. **
 41 1 1. *END*

EQUIPMENT PARAMETER SPECIFICATIONS

1 7, 2 6, 3 1, 4 5, 5 4, 6 3, 7 4, 8 2, 9 5, 10 3, 11 4,
 12 8, 13 9, 14 6 **
 1 1 2. 2 45. 3 75. 4 18.5 5 1. 6 0.3333 **
 2 1 0.1 2 5. **
 3 1 3. 3 1. 10 900. 11 600. 13 0.6 14 0.9 15 0.6

PROGRAM DATA (CARD IMAGE)

```

19 0.2 20 7. 25 1600.  **
4 1 450. 3 7.  **
5 1 1. 7 9. 10 25.  **
6 1 1. 8 0.15  **
7 1 2. 7 13. 10 13.  **
8 4 5E4  **
9 1 425. 3 14.  **
10 1 2. 8 0.15  **
11 1 3. 7 18. 10 4.  **
12 1 1250. 2 55. 3 80. 4 15. 5 1.25 6 1.0 7 19.  **
13 1 75. 2 1175. 5 0.2 6 80.  **  *END*
*MOLECULAR AND THERMODYNAMIC DATA***
'H' 1.,3.7  'C' 12.,14.8  'O' 16.,7.4  'S' 32.,25.6
'N' 14. 15.6  **
  'CH4 '
+4.2497678E+00 -6.9126562E-03 +3.1602134E-05 -2.9715432E-08
+9.5103580E-12 -1.0186632E+04 -9.1754991E-01
+1.1795744E+00 +1.0950594E-02 -4.0622131E-06 +7.1370281E-10
-4.7490353E-14 -9.8556627E+03 +1.2505934E+01  **
  'CO2 ' , 0.0135, 0.0000205
+2.1701000E+00 +1.0378115E-02 -1.0733938E-05 +6.3459175E-09
-1.6280701E-12 -4.8352602E+04 +1.0664388E+01
+4.4129266E+00 +3.1922896E-03 -1.2978230E-06 +2.4147446E-10
-1.6742986E-14 -4.8944043E+04 -7.2875769E-01  **
  'O2 G' 0.02, 0.00002
+3.7189946E+00 -2.5167288E-03 +8.5837353E-06 -8.2998716E-09
+2.7082180E-12 -1.0576706E+03 +3.9080704E+00
+3.5976129E+00 +7.8145603E-04 -2.2386670E-07 +4.2490159E-11
-3.3460204E-15 -1.1927918E+03 +3.7492659E+00  **
  'N2 ' , 'G', 0.0175 , 0.0000195
+3.6916148E+00 -1.3332552E-03 +2.6503100E-06 -9.7688341E-10
-9.9772234E-14 -1.0628336E+03 +2.2874980E+00
+2.8545761E+00 +1.5976316E-03 -6.2566254E-07 +1.1315849E-10
-7.6897070E-15 -8.9017445E+02 +6.3902879E+00  **
  'H2O ' 'G', 0.008, 0.000021
+4.1565016E+00 -1.7244334E-03 +5.6982316E-06 -4.5930044E-09
+1.4233654E-12 -3.0288770E+04 -6.8616246E-01
+2.6707532E+00 +3.0317115E-03 -8.5351570E-07 +1.1790853E-10
-6.1973568E-15 -2.9388994E+04 +6.8838391E+00  **
  'H2S ' 'G', 0.011 0.000024
+3.9163074E+00 -3.5138671E-04 +4.2191312E-06 -2.7453665E-09
+4.3584365E-13 -3.6095585E+03 +2.3660042E+00
+2.7657149E+00 +4.0131914E-03 -1.5044898E-06 +2.6807998E-10
-1.7967681E-14 -3.3359808E+03 +7.9327186E+00  **
  'SO2 ' 'G' .0115 .000017
+3.2257132E+00 +5.6551207E-03 -2.4970208E-07 -4.2206766E-09
+2.1392733E-12 -3.6904476E+04 +9.8177036E+00
+5.1982451E+00 +2.0595095E-03 -8.6254450E-07 +1.6636523E-10

```


PROGRAM DATA (CARD IMAGE)

```

-1.1847837E-14 -3.7541457E+04 -8.3059963E-01      **
      'S'      'G'
+2.9137258E+00 +3.1294061E-04 -2.6092508E-06 +3.1382439E-09
-1.1708988E-12 +3.2568272E+04 +3.5681154E+00
+2.9145770E+00 -5.6619390E-04 +2.8497584E-07 -5.1868520E-11
+3.2709932E-15 +3.2604940E+04 +3.7640850E+00      **
      'S2'     'G'
+2.6999349E+00 +6.2749549E-03 -9.2870775E-06 +6.5393276E-09
-1.7802282E-12 +1.4504935E+04 +1.0534222E+01
+4.1896932E+00 +3.8469704E-04 -1.5566633E-07 +3.0368010E-11
-2.1795849E-15 +1.4188133E+04 +3.2930300E+00      **
      'S6'     'G'
+6.0892429E+00 +1.8824865E-02 -2.7861233E-05 +1.9617983E-08
-5.3406846E-12 +1.1264370E+04 +7.3202322E+00
+1.0558515E+01 +1.1540911E-03 -4.6699899E-07 +9.1104030E-11
-6.5387547E-15 +1.0313964E+04 -1.4403344E+01      **
      'S8'     'G'
+7.7838968E+00 +2.5099820E-02 -3.7148310E-05 +2.6157310E-08
-7.1209128E-12 +1.0114584E+04 +4.7621792E+00
+1.3742926E+01 +1.5387882E-03 -6.2266532E-07 +1.2147204E-10
-8.7183396E-15 +8.8473760E+03 -2.4202589E+01      **
      'COS G'
+2.0885523E+00 +1.4613989E-02 -2.0465884E-05 +1.5062439E-08
-4.4468532E-12 -1.7624238E+04 +1.2367372E+01
+5.2068373E+00 +2.4717661E-03 -1.0011287E-06 +1.8787369E-10
-1.3103525E-14 -1.8327771E+04 -2.9133806E+00      **
      'CS2 G'      .17 .000017
+2.9174620E+00 +1.2498700E-02 -1.6109132E-05 +1.0567832E-08
-2.7944978E-12 +1.2777076E+04 +8.8763481E+00
+5.9491526E+00 +1.7245610E-03 -7.2111106E-07 +1.3744760E-10
-9.6838965E-15 +1.2053749E+04 -6.2051076E+00      **
      'H2 G' 0.008 .0000085
+2.8460849E+00 +4.1932116E-03 -9.6119332E-06 +9.5122662E-09
-3.3093421E-12 -9.6725372E+02 -1.4117850E+00
+3.0436897E+00 +6.1187110E-04 -7.3993551E-09 -2.0331907E-11
+2.4523791E-15 -8.5491002E+02 -1.6481339E+00      **
      'CD G' .017 .0000175
+3.7871332E+00 -2.1709526E-03 +5.0757337E-06 -3.4737726E-09
+7.7216841E-13 -1.4363508E+04 +2.6335459E+00
+2.9511519E+00 +1.5525567E-03 -6.1911411E-07 +1.1350336E-10
-7.7882732E-15 -1.4231827E+04 +6.5314450E+00      **
      'S L'
-4.1562591E+01 +2.8300951E-01 -6.2124646E-04 +5.7917986E-07
-1.9550879E-10 +4.4720883E+03 1.7978686E+02 3.8716625
0. 0. 0. 0. -8.4632533E+02 -1.7492768E+01      **

```

END OF ALL DATA

SULPHUR PLANT DESIGN AND SIMULATION

PROGRAM CONTROL PARAMETERS

ECHO CHECK OF PROGRAM CONTROL PARAMETERS

PRINT SUPPRESS

VALUE OF THE CALCULATIONAL CRITERION IS $0.10E-03$
(ALL INTERNAL CONVERGENCE CRITERIA ETC. ARE SCALED TO THIS)

IDBUG	VALUE	APPLICATION
1	1	WASTE HEAT BOILER
2	1	IN-LINE BURNER
3	1	CONVERTER
4	1	CONDENSER
5	1	ADIABATIC COMBINER
6	1	COMBINER/DIVIDER
7	1	COMBUSTION AIR ADDER
8	1	INCINERATOR
9	1	STACK
10	1	BLACK BOX
11	0	
12	0	EQUILIBRIUM COMPOSITION
13	0	CALCULATION OPTIMIZATION
14	5	DATA INPUT ECHO CHECK
15	1	EXECUTIVE FUNCTIONS

END

FLOWSHEET DATA

ECHO CHECK OF FLOWSHEET DATA

STREAM NUMBER	SOURCE EQUIP. NO.	DESTINATION EQUIP. NO.	STREAM UNKNOWN	STREAM FLAG
1	0	1	1	0
2	0	1	1	0
3	1	2	1	0
4	2	3	1	0
5	2	8	1	0
6	3	5	1	0
7	3	4	1	0
8	5	4	1	0
9	5	14	1	0
10	4	6	1	0
11	6	7	1	0
12	7	9	1	0
13	7	14	1	0
14	8	9	1	0
15	9	10	1	0
16	10	11	1	0
17	11	12	1	0
18	11	14	1	0
19	0	12	1	0
20	12	13	1	0
21	13	0	1	0
22	14	0	1	0
30	0	3	0	1
31	3	0	0	1
32	0	5	0	1
33	5	0	0	1
34	0	7	0	1
35	7	0	0	1
36	0	11	0	1
37	11	0	0	1
40	4	3	1	-1
41	9	2	1	-1

END

STREAM SPECIFICATIONS

ECHO CHECK OF STREAM SPECIFICATION DATA

STREAM - ' (PARAMETER NO.)PARAMETER VALUE' REPEATED

- 1 - (1) 0.15677E 01 (2) 0.10429E 03 (5) 0.47000E 02
 (6) 0.29004E 03 (21) 0.70000E 02 (22) 0.19000E 02

- 19 - (1) 0.20910E 02 (21) 0.10000E 03 (22) 0.13000E 02

- 40 - (1) 0.19000E 02

- 41 - (1) 0.10000E 01

END

EQUIPMENT PARAMETER SPECIFICATIONS

ECHO CHECK OF EQUIPMENT PARAMETER SPECIFICATION DATA

EQUIP. NO.	-	1	2	3	4	5	6	7	8	9	10
		11	12	13	14						
EQUIP. TYPE	-	7	6	1	5	4	3	4	2	5	3
		4	8	9	6						
EQUIP. INDEX	-	0	6	8	36	39	51	59	71	76	79
		87	99	106	114						

EQUIPMENT
NUMBER

PARAMETER
NUMBER

PARAMETER
VALUE

1	1	0.2000000E 01
	2	0.4500000E 02
	3	0.7500000F 02
	4	0.1850000E 02
	5	0.1000000E 01
	6	0.3332999E 00
2	1	0.9999996E-01
	2	0.5000000F 01
3	1	0.3000000E 01
	3	0.1000000E 01
	10	0.9000000E 03
	11	0.6000000E 03
	13	0.6000000E 00
	14	0.9000000F 00
	15	0.6000000F 00
	19	0.2000000E 00
	20	0.7000000E 01
	25	0.1600000E 04
4	1	0.4500000E 03
	3	0.7000000E 01
5	1	0.1000000E 01
	7	0.9000000E 01
	10	0.2500000E 02
6	1	0.1000000E 01
	8	0.1499999E 00

EQUIPMENT NUMBER	PARAMETER NUMBER	PARAMETER VALUE
7	1	0.2000000F 01
	7	0.1300000E 02
	10	0.1300000E 02
8	4	0.5000000F 05
9	1	0.4250000E 03
	3	0.1400000E 02
10	1	0.2000000E 01
	8	0.1499999E 00
11	1	0.3000000F 01
	7	0.1800000E 02
	10	0.4000000E 01
12	1	0.1250000E 04
	2	0.5500000E 02
	3	0.8000000E 02
	4	0.1500000E 02
	5	0.1249999E 01
	6	0.1000000E 01
	7	0.1900000E 02
13	1	0.7500000E 02
	2	0.1175000E 04
	5	0.2000000F 00
	6	0.8000000E 02

END

MOLECULAR AND THERMODYNAMIC DATA

ECHO CHECK OF MOLECULAR AND THERMODYNAMIC DATA

ATOM -

NAME	H	C	O	S	N
WEIGHT	1.00	12.00	16.00	32.00	14.00
VOLUME	3.70	14.80	7.40	25.60	15.60

SPECIE	*	MOLECULAR	*	* VISCOSITY *		
NUMBER	FORMULA	WEIGHT	VOLUME	RADCT	RMU	SMU

1	CH4	G	16.0	29.6	1.0	0.0150	0.0000200	*
2	CO2	G	44.0	29.6	1.0	0.0135	0.0000205	
3	O2	G	32.0	14.8	0.0	0.0200	0.0000200	
4	N2	G	28.0	31.2	0.0	0.0175	0.0000195	
5	H2O	G	18.0	14.8	1.0	0.0080	0.0000210	
6	H2S	G	34.0	33.0	1.0	0.0110	0.0000240	
7	SO2	G	64.0	40.4	1.0	0.0115	0.0000170	
8	S	G	32.0	25.6	0.0	0.0150	0.0000200	*
9	S2	G	64.0	51.2	0.0	0.0150	0.0000200	*
10	S6	G	192.0	153.6	1.0	0.0150	0.0000200	*
11	S8	G	256.0	204.8	1.0	0.0150	0.0000200	*
12	COS	G	60.0	47.8	1.0	0.0150	0.0000200	*
13	CS2	G	76.0	66.0	1.0	0.1700	0.0000170	
14	H2	G	2.0	7.4	0.0	0.0080	0.0000085	
15	CO	G	28.0	22.2	0.0	0.0170	0.0000175	
16	S	L	32.0	0.0	0.0	0.0150	0.0000200	*

VISCOSITY DATA IN FORM - MU(CP)=RMU+SMU*T DEG. F.
* DENOTES ASSUMED VISCOSITY CONSTANTS

WATER COMPONENT = 5 SULPHUR COMPONENTS = 8 9 10 11 16

THERMODYNAMIC DATA - NASA FORMAT
 FIRST 7 CONSTANTS FOR 300 TO 1000 DEG. K.
 LAST 7 CONSTANTS FOR 1000 TO 5000 DEG. K.

CH4	0.4249765E 01	-0.6912652E-02	0.3160210E-04
-0.2971539E-07	0.9510352E-11	-0.1018660E 05	-0.9175493E 00
0.1179572E 01	0.1095056E-01	-0.4062208E-05	0.7137024E-09
-0.4749034E-13	-0.9855656E 04	0.1250591E 02	

CO2	0.2170098E 01	0.1037809E-01	-0.1073391E-04
0.6345910E-08	-0.1628067E-11	-0.4835256E 05	0.1066436E 02
0.4412923E 01	0.3192285E-02	-0.1297819E-05	0.2414740E-09
-0.1674295E-13	-0.4894401E 05	-0.7287572E 00	

O2	0.3718991E 01	-0.2516725E-02	0.8583728E-05
-0.8299864E-08	0.2708214E-11	-0.1057668E 04	0.3908069E 01
0.3597610E 01	0.7814555E-03	-0.2238664E-06	0.4249015E-10
-0.3346017E-14	-0.1192789E 04	0.3749263E 01	

N2	0.3691611E 01	-0.1333252E-02	0.2650306E-05
-0.9768830E-09	-0.9977219E-13	-0.1062831E 04	0.2287497E 01
0.2854573E 01	0.1597629E-02	-0.6256620E-06	0.1131581E-09
-0.7689704E-14	-0.8901741E 03	0.6390284E 01	

H2O	0.4156499E 01	-0.1724431E-02	0.5698224E-05
-0.4593002E-08	0.1423361E-11	-0.3028874E 05	-0.6861618E 00
0.2670752E 01	0.3031709E-02	-0.8535151E-06	0.1179083E-09
-0.6197350E-14	-0.2988896E 05	0.6883836E 01	

H2S	0.3916305E 01	-0.3513861E-03	0.4219126E-05
-0.2745363E-08	0.4853431E-12	-0.3609556E 04	0.2366002E 01
0.2765712E 01	0.4013184E-02	-0.1504486E-05	0.2680796E-09
-0.1796765E-13	-0.3385977E 04	0.7932716E 01	

SO2	0.3225711E 01	0.5655114E-02	-0.2497017E-06
-0.4220674E-08	0.2139270E-11	-0.3690444E 05	0.9817701E 01
0.5198241E 01	0.2059507E-02	-0.8625439E-06	0.1663650E-09
-0.1184781E-13	-0.3754142E 05	-0.3305990E 00	

S	0.2913722E 01	0.3129402E-03	-0.2609247E-05
0.3138239E-08	-0.1170895E-11	0.3256823E 05	0.3568112E 01
0.2914575E 01	-0.5661934E-03	0.2849755E-06	-0.5186851E-10
0.3270991E-14	0.3260492E 05	0.3764083E 01	

S2	0.2699931E 01	0.6274950E-02	-0.9287070E-05
0.6539324E-08	-0.1780224E-11	0.1450491E 05	0.1053419E 02
0.4189692E 01	0.3846965E-03	-0.1556660E-06	0.3036800E-10
-0.2179581E-14	0.1413810E 05	0.3293028E 01	

S6	0.6089240E 01	0.1382483E-01	-0.2786120E-04
0.1961795E-07	-0.5340679E-11	0.1126434E 05	0.7320230E 01
0.1055848E 02	0.1154089E-02	-0.4669984E-06	0.9110405E-10
-0.6538749E-14	0.1031394E 05	-0.1440332E 02	

THERMODYNAMIC DATA - NASA FORMAT
 FIRST 7 CONSTANTS FOR 300 TO 1000 DEG. K.
 LAST 7 CONSTANTS FOR 1000 TO 5000 DEG. K.

S8	0.7783894E 01	0.2509980E-01	-0.3714827E-04
0.2615727E-07	-0.7120906E-11	0.1011455E 05	0.4762177E 01
0.1374290E 02	0.1538786E-02	-0.6226649E-06	0.1214713E-09
-0.8718334E-14	0.8847371E 04	-0.2420255E 02	

CDS	0.2088551E 01	0.1461395E-01	-0.2046586E-04
0.1506240E-07	-0.4446848E-11	-0.1762420E 05	0.1236735E 02
0.5206835E 01	0.2471763E-02	-0.1001124E-05	0.1878734E-09
-0.1310349E-13	-0.1832775E 05	-0.2913377E 01	

CS2	0.2917459E 01	0.1249868E-01	-0.1610910E-04
0.1056780E-07	-0.2794493E-11	0.1277706E 05	0.8876345E 01
0.5949150E 01	0.1724559E-02	-0.7211104E-06	0.1374474E-09
-0.9683891E-14	0.1205371E 05	-0.6205195E 01	

H2	0.2846082E 01	0.4193205E-02	-0.9611924E-05
0.9512259E-08	-0.3309338E-11	-0.9672534E 03	-0.1411782E 01
0.3043687E 01	0.6118708E-03	-0.7399350E-08	-0.2033189E-10
0.2459376E-14	-0.8549097E 03	-0.1648130E 01	

CO	0.3787131E 01	-0.2170950E-02	0.5075728E-05
-0.3473769E-08	0.7721680E-12	-0.1436348E 05	0.2633542E 01
0.2951148E 01	0.1552554E-02	-0.6191135E-06	0.1135031E-09
-0.7788268E-14	-0.1423179E 05	0.6531443E 01	

S	-0.4156255E 02	0.2830092E 00	-0.6212459E-03
0.5791794E-06	-0.1955084E-09	0.4472086E 04	0.1797865E 03
0.3871659E 01	0.0	0.0	0.0
0.0	-0.8463250E 03	-0.1749274E 02	

END OF ALL DATA

CALCULATION SEQUENCE OPTIMIZATION

INITIAL SEQUENCE IS -

1 2 3 4 5 6 7 8 9 10 11 12 13 14

THE OPTIMIZED CALCULATION SEQUENCE IS -

1 2 8 3 5 4 6 7 9 10 11 14 12 13

THE FOLLOWING STREAMS MUST BE ASSUMED,

41 40

PRIMARY REACTION CUT-OFF TEMPERATURE (BOILER) = 1600. DEG.F

COMBUSTION AIR ADDER
EQUIPMENT NUMBER 1

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 70.0 PRESSURE (PSIA) = 19.00
STREAM ENTHALPY (BTU.) = -0.2513813E 08

MOLE NUMBERS ARE -

CH4	-	1.56770	CO2	-	104.29167
O2	-	0.0	N2	-	0.0
H2O	-	47.00000	H2S	-	290.04126
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	0.0

TOTAL MOLES AIR ADDED = 712.85 (R.H. = 45.00 PERCENT)
MOLES DRY AIR = 705.43 MOLES WATER = 7.42
TEMPERATURE (DEG.F.) = 75.0 PRESSURE (PSIA.) = 18.50

RATIO OF (SPECIFIED/STOICHIOMETRIC) AIR ADDED -

- FOR OXIDATION OF SULPHUR (ALL H2S) - 0.3333
- FOR OXIDATION OF CARBON, HYDROGEN AND ABOVE - 1.0000

COMBINED OUTLET STREAM
STREAM NUMBER 3

TEMPERATURE (DEG. F) = 72.9 PRESSURE (PSIA) = 18.50
STREAM ENTHALPY (BTU.) = -0.2591994E 08

MOLE NUMBERS ARE -

CH4	-	1.56770	CO2	-	104.29167
O2	-	148.14136	N2	-	557.29346
H2O	-	54.42023	H2S	-	290.04126
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	0.0

STREAM COMBINER / DIVIDER
EQUIPMENT NUMBER 2

INLINE BURNER.
EQUIPMENT NUMBER 8

COMBUSTION REACTION AND WASTE HEAT BOILER.
EQUIPMENT NUMBER 3

CONDENSER 1
EQUIPMENT NUMBER 5

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 4

CONVERTER 1
EQUIPMENT NUMBER 6

CONDENSER 2
EQUIPMENT NUMBER 7

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 9

CALCULATIONS LOOPED ON RECYCLE LOOP -

2 8 3 5 4 6 7 9

STREAM COMBINER / DIVIDER
EQUIPMENT NUMBER 2

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 72.9 PRESSURE (PSIA) = 18.50
STREAM ENTHALPY (BTU.) = -0.2591994E 08

MOLE NUMBERS ARE -

CH4	-	1.56770	CO2	-	104.29167
O2	-	148.14136	N2	-	557.29346
H2O	-	54.42023	H2S	-	290.04126
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	0.0

TOTAL FEED IS SPLIT -

3.054 PERCENT TO STREAM 5 ,
96.946 PERCENT TO STREAM 4

INLINE BURNER.
EQUIPMENT NUMBER 8

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 72.9 PRESSURE (PSIA) = 18.50
STREAM ENTHALPY (BTU.) = -0.7915135E 06

MOLE NUMBERS ARE -

CH4	-	0.04787	CO2	-	3.18474
O2	-	4.52377	N2	-	17.01799
H2O	-	1.66182	H2S	-	8.85695
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	0.0

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 2010.2 DEG. F
PRESSURE (PSIA.) = 18.50 (CRIT = 0.10E-03)

IN-LINE BURNER -

(DESIGN)

DIAMETER (IN.) = 24.0 RESIDENCE TIME (SEC.) = 2.245
LENGTH (FT.) = 10.0 HEAT RELEASE (BTU/CU.FT.) = 18945.

BURNER EXIT STREAM -
STREAM NUMBER 14

TEMPERATURE (DEG. F) = 2010.2 PRESSURE (PSIA) = 18.50
STREAM ENTHALPY (BTU.) = -0.7915126E 06

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	2.77810
O2	-	0.00000	N2	-	17.01799
H2O	-	8.47096	H2S	-	1.51392
SO2	-	1.29863	S	-	0.00007
S2	-	3.00688	S6	-	0.00000
S8	-	0.0	COS	-	0.03043
CS2	-	0.00009	H2	-	0.62964
CO	-	0.42400	S	-	0.0

COMBUSTION REACTION AND WASTE HEAT BOILER.
EQUIPMENT NUMBER 3

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 72.9 PRESSURE (PSIA) = 18.50
STREAM ENTHALPY (BTU.) = -0.2512842E 08

MOLE NUMBERS ARE -

CH4	-	1.51983	CO2	-	101.10693
O2	-	143.61758	N2	-	540.27539
H2O	-	52.75339	H2S	-	281.18408
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	0.0

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 2010.2 DEG. F
PRESSURE (PSIA.) = 18.50 (CRIT = 0.10E-03)

STREAM ENTHALPY (BTU.) = -0.2512808E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	88.19630
O2	-	0.00000	N2	-	540.27539
H2O	-	268.93018	H2S	-	48.06148
SO2	-	41.22824	S	-	0.00220
S2	-	95.46013	S6	-	0.00000
S8	-	0.0	COS	-	0.96594
CS2	-	0.00294	H2	-	19.98988
CO	-	13.46154	S	-	0.0

BOILER FIRE TUNNEL - (DESIGN)

DIAMETER (IN.) = 60.0 RESIDENCE TIME (SEC.) = 0.884
LENGTH (FT.) = 20.0 HEAT RELEASE (BTU/CU.FT.) = 48117.

SIMULATION OF TUBE PASS NO. 1

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 1672.1 DEG. F
PRESSURE (PSIA.) = 18.50 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 60.00
NUMBER OF TUBES = 1.
TUBE LENGTH (FT.) = 20.00
PRESSURE DROP (PSI) = 0.00
TOTAL HEAT LOSS (BTU.) = 0.4548236E 07
STREAM ENTHALPY (BTU.) = -0.2967659E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	97.96252
O2	-	0.0	N2	-	540.27539
H2O	-	265.50317	H2S	-	63.69708
SO2	-	38.05815	S	-	0.00010
S2	-	89.26601	S6	-	0.00009
S8	-	0.00000	COS	-	0.89133
CS2	-	0.00234	H2	-	7.78099
CO	-	3.77051	S	-	0.0

DESIGN OF PASS NO. 2

ITERATIVE CALCULATION OF TUBE-PASS TUBE-NUMBER
TDIAM SPECIFIED, DELPC CALCULATED.

CONVERGED TUBE NUMBER IS 89.
TUBE DIAMETER (IN) IS 2.50
TUBE LENGTH (FT) IS 20.00

APPROX. PRESS. DROP (PSI.) = 0.18
APPROX. TOTAL HEAT LOSS (BTU.) = 0.1064743E 08
(FNTH. ERROR (BTU.) = 0.4400000E 02)

REVERT TO SIMULATION FOR EXACT CALCULATION
OF ACTUAL OUTLET TEMP. AND PRESS. DROP

SIMULATION OF TUBE PASS NO. 2

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 900.4 DEG. F
PRESSURE (PSIA.) = 18.31 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 2.50
NUMBER OF TUBES = 89.
TUBE LENGTH (FT.) = 20.00
PRESSURE DROP (PSI) = 0.19
TOTAL HEAT LOSS (BTU.) = 0.1063464E 08

STREAM ENTHALPY (BTU.) = -0.4030520E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	99.13789
O2	-	0.0	N2	-	540.27539
H2O	-	263.76416	H2S	-	67.19925
SO2	-	38.33974	S	-	0.00000
S2	-	22.04135	S6	-	17.48224
S8	-	3.22716	COS	-	0.84644
CS2	-	0.00211	H2	-	6.01762
CO	-	2.64024	S	-	0.0

BOILER BY-PASS NO. 1 , (RATIO = 0.12321)
STREAM NUMBER 7

TEMPERATURE (DEG. F) = 900.4 PRESSURE (PSIA) = 18.31
STREAM ENTHALPY (BTU.) = -0.4964765E 07

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	12.21173
O2	-	0.0	N2	-	66.55067
H2O	-	32.49025	H2S	-	8.27755
SO2	-	4.72266	S	-	0.00000
S2	-	2.71504	S6	-	2.15345
S8	-	0.39752	COS	-	0.10426
CS2	-	0.00026	H2	-	0.74125
CO	-	0.32522	S	-	0.0

DESIGN OF PASS NO. 3

ITERATIVE CALCULATION OF TUBE-PASS TUBE-NUMBER
TDIAM SPECIFIED, DELPC CALCULATED.

CONVERGED TUBE NUMBER IS 74.
TUBE DIAMETER (IN) IS 2.00
TUBE LENGTH (FT) IS 20.00

APPROX. PRESS. DROP (PSI.) = 0.37
APPROX. TOTAL HEAT LOSS (BTU.) = 0.3367155E 07
(ENTH. ERROR (BTU.) = 0.2445000E 04)

REVERT TO SIMULATION FOR EXACT CALCULATION
OF ACTUAL OUTLET TEMP. AND PRESS. DROP

SIMULATION OF TUBE PASS NO. 3

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 599.4 DEG. F
PRESSURE (PSIA.) = 17.95 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 2.00
NUMBER OF TUBES = 74.
TUBE LENGTH (FT.) = 20.00
PRESSURE DROP (PSI) = 0.37
TOTAL HEAT LOSS (BTU.) = 0.3371565E 07

BOILER EXIT STREAM -
STREAM NUMBER 6

TEMPERATURE (DEG. F) = 599.4 PRESSURE (PSIA) = 17.95
STREAM ENTHALPY (BTU.) = -0.3871123E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	86.92036
O2	-	0.0	N2	-	473.72461
H2O	-	231.33430	H2S	-	58.84355
SO2	-	33.58974	S	-	0.0
S2	-	0.25076	S6	-	10.26678
S8	-	11.40837	COS	-	0.74095
CS2	-	0.00184	H2	-	5.29410
CO	-	2.32204	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 514.9
STREAM WATER DEW PT. (DEG. F) = 158.2

EQUIP. HEAT DUTY (BTU/HR) IS 0.1855443E 08

STEAM TEMP. (DEG. F.) = 401.0
PRESS. (PSIA) = 250.000
LATENT HEAT (BTU/LB) = 822.1
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.2257018E 05

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 62.20

CONDENSER 1
EQUIPMENT NUMBER 5

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 599.4 PRESSURE (PSIA) = 17.95
STREAM ENTHALPY (BTU.) = -0.3871123E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	86.92036
O2	-	0.0	N2	-	473.72461
H2O	-	231.33430	H2S	-	58.84355
SO2	-	33.58974	S	-	0.0
S2	-	0.25076	S6	-	10.26678
S8	-	11.40837	COS	-	0.74095
CS2	-	0.00184	H2	-	5.29410
CO	-	2.32204	S	-	0.0

CONDENSER DESIGN

TUBE LENGTH (FT.) = 10.7
TUBE DIAMETER (IN.) = 1.000
NUMBER OF TUBES = 387

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.00
OUTLET GAS TEMPERATURE (DEG.F) = 364.9
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 13.52

EQUIP. HEAT DUTY (BTU/HR) IS 0.2583712E 07

STEAM TEMP. (DEG.F.) = 281.1
PRESS. (PSIA) = 50.000
LATENT HEAT (BTU/LB) = 924.7
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.2794053E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 94.66, PERCENT RECOVERY = 42.68

SULPHUR FOG - 79.73 MOLES, OR 2551.4 LBS.
SULPHUR LIQUID - 65.45 MOLES, OR 2094.5 LBS.
(STREAM NO. 9 , TEMPERATURE = 293.1 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INFRTS) = 25.00

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 94.66, PERCENT RECOVERY = 90.11

SULPHUR FOG - 6.97 MOLES, OR 223.2 LBS.
SULPHUR LIQUID - 138.21 MOLES, OR 4422.6 LBS.
(STREAM NO. 9 , TEMPERATURE = 331.4 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 8

TEMPERATURE (DEG. F) = 364.9 PRESSURE (PSIA) = 17.84
STREAM ENTHALPY (BTU.) = -0.4165973E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	86.92036
O2	-	0.0	N2	-	473.72461
H2O	-	231.33430	H2S	-	58.84355
SO2	-	33.58974	S	-	0.0
S2	-	0.00033	S6	-	0.23105
S8	-	0.84999	COS	-	0.74095
CS2	-	0.00184	H2	-	5.29410
CO	-	2.32204	S	-	6.97478

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 4

COMBINE STREAMS 7 AND 8

FIND GIVEN FEED STREAM RESULTANT TEMPERATURE
ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 450.1 DEG. F
PRESSURE (PSIA.) = 17.84 (CRIT = 0.10E-03)

PREDICTED STREAM SPLIT FOR TEMP. OF 450.0000 IS 0.1232
USE STREAMS RESULTING FROM THIS PREDICTION
FOR PRESENT EQUIPMENT OUTLET STREAM.

COMBINED OUTLET STREAM (SULPHUR SHIFT DONE) -
STREAM NUMBER 10

TEMPERATURE (DEG. F) = 450.0 PRESSURE (PSIA) = 17.84
STREAM ENTHALPY (BTU.) = -0.4662562E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	99.13208
O2	-	0.0	N2	-	540.27515
H2O	-	263.82446	H2S	-	67.12109
SO2	-	38.31239	S	-	0.0
S2	-	0.00643	S6	-	1.49281
S8	-	3.46535	COS	-	0.84522
CS?	-	0.00210	H2	-	6.03534
CO	-	2.64726	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 425.8
STREAM WATER DEW PT. (DEG. F) = 158.8

CONVERTER 1
EQUIPMENT NUMBER 6

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 450.0 PRESSURE (PSIA) = 17.84
STREAM ENTHALPY (BTU.) = -0.4662562E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	99.13208
O2	-	0.0	N2	-	540.27515
H2O	-	263.82446	H2S	-	67.12109
SO2	-	38.31239	S	-	0.0
S2	-	0.00643	S6	-	1.49281
S8	-	3.46535	COS	-	0.84522
CS2	-	0.00210	H2	-	6.03534
CO	-	2.64726	S	-	0.0

CONVERTER BED (DESIGN)

CROSSECTIONAL AREA (SQ.FT) = 161.60
THICKNESS (FT.) = 3.00
VOLUME (CU.FT.) = 484.79
LINEAR GAS VELOCITY (FT./SEC.) = 1.00
MOLAL FLOW RATE (MOLF/HR.SQ.FT.) = 2.11
AVERAGE PARTICLE DIAMETER (IN.) = 0.15
PRESSURE DROP (PSI.) = 0.451

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 609.6 DEG. F
PRESSURE (PSIA.) = 17.39 (CRIT = 0.10E-03)

CONVERTER DEW POINT CHECK -

BED TEMPERATURE	DEW POINT TEMPERATURE	TEMPERATURE DIFFERENCE	BED PRESSURE
481.924	443.112	38.812	17.749
513.848	456.903	56.945	17.659
545.772	468.558	77.214	17.568
577.696	478.800	98.896	17.478
609.620	488.063	121.556	17.388

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 77.24

PERCENT OF NON-ELEMENTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 69.39

CONVERTER EXIT STREAM -
STREAM NUMBER 11

TEMPERATURE (DEG. F) = 609.6 PRESSURE (PSIA) = 17.39
STREAM ENTHALPY (BTU.) = -0.4662570E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	102.61899
O2	-	0.0	N2	-	540.27515
H2O	-	315.28247	H2S	-	21.69176
SO2	-	10.83838	S	-	0.0
S2	-	0.30416	S6	-	8.26060
S8	-	7.53322	COS	-	0.00757
CS2	-	0.00000	H2	-	0.00564
CO	-	0.00006	S	-	0.0

CONDENSER 2
EQUIPMENT NUMBER 7

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 609.6 PRESSURE (PSIA) = 17.39
STREAM ENTHALPY (BTU.) = -0.4662570E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	102.61899
O2	-	0.0	N2	-	540.27515
H2O	-	315.28247	H2S	-	21.69176
SO2	-	10.83838	S	-	0.0
S2	-	0.30416	S6	-	8.26060
S8	-	7.53322	COS	-	0.00757
CS2	-	0.00000	H2	-	0.00564
CO	-	0.00006	S	-	0.0

CONDENSER DESIGN

TUBE LENGTH (FT.) = 11.9
TUBE DIAMETER (IN.) = 1.000
NUMBER OF TUBES = 386

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.00
OUTLET GAS TEMPERATURE (DEG.F) = 347.5
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 13.99

EQUIP. HEAT DUTY (BTU/HR) IS 0.2750571E 07

STEAM TEMP. (DEG.F.) = 281.1
PRESS. (PSIA) = 50.000
LATENT HEAT (BTU/LB) = 924.7
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.2974496E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 94.54, PERCENT RECOVERY = 47.01
SULPHUR FOG - 52.49 MOLES, OR 1679.8 LBS.
SULPHUR LIQUID - 51.92 MOLES, OR 1661.4 LBS.
(STREAM NO. 13 , TEMPERATURE = 291.5 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INEPTS) = 13.00

EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 94.54, PERCENT RECOVERY = 90.90
SULPHUR FOG - 4.02 MOLES, OR 128.8 LBS.
SULPHUR LIQUID - 100.39 MOLES, OR 3212.4 LBS.
(STREAM NO. 13 , TEMPERATURE = 318.9 DEG.F.)

CONDENSER GASFOUS EXIT STREAM
STREAM NUMBER 12

TEMPERATURE (DEG. F) = 347.5 PRESSURE (PSIA) = 17.25
STREAM ENTHALPY (BTU.) = -0.4963032F 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	102.61899
O2	-	0.0	N2	-	540.27515
H2O	-	315.28247	H2S	-	21.69176
SO2	-	10.83838	S	-	0.0
S2	-	0.00019	S6	-	0.16038
S3	-	0.63283	COS	-	0.00757
CS2	-	0.00000	H2	-	0.00564
CO	-	0.00006	S	-	4.02480

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 9

COMBINE STREAMS 12 AND 14

FIND GIVEN FEED STREAM RESULTANT TEMPERATURE
ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 425.0 DEG. F
PRESSURE (PSIA.) = 17.25 (CRIT = 0.10F-03)

PREDICTED STREAM SPLIT FOR TEMP. OF 425.0000 IS 0.0305
USE STREAMS RESULTING FROM THIS PREDICTION
FOR PRESENT EQUIPMENT OUTLET STREAM.

COMBINED OUTLET STREAM (SULPHUR SHIFT DONE) -
STREAM NUMBER 15

TEMPERATURE (DEG. F) = 425.0 PRESSURE (PSIA) = 17.25
STREAM ENTHALPY (BTU.) = -0.5042186E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	105.39708
O2	-	0.00000	N2	-	557.29297
H2O	-	323.75342	H2S	-	23.20567
SO2	-	12.13701	S	-	0.0
S2	-	0.00268	S6	-	0.65444
S8	-	1.51649	COS	-	0.03800
CS2	-	0.00009	H2	-	0.63529
CO	-	0.42406	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 386.5
STREAM WATER DEW PT. (DEG. F) = 165.9

CONVERTER 2
EQUIPMENT NUMBER 10

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 425.0 PRESSURE (PSIA) = 17.25
STREAM ENTHALPY (BTU.) = -0.5042186E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	105.39708
O2	-	0.00000	N2	-	557.29297
H2O	-	323.75342	H2S	-	23.20567
SO2	-	12.13701	S	-	0.0
S2	-	0.00268	S6	-	0.65444
S8	-	1.51649	COS	-	0.03800
CS2	-	0.00009	H2	-	0.63529
CO	-	0.42406	S	-	0.0

CONVERTER BED (DESIGN)

CROSSECTIONAL AREA (SQ.FT) = 163.04
THICKNESS (FT.) = 3.00
VOLUME (CU.FT.) = 489.13
LINEAR GAS VELOCITY (FT./SEC.) = 1.00
MOLAL FLOW RATE (MOLE/HR.SQ.FT.) = 2.10
AVERAGE PARTICLE DIAMETER (IN.) = 0.15
PRESSURE DROP (PSI.) = 0.383

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 473.0 DEG. F
PRESSURE (PSIA.) = 16.86 (CRIT = 0.10E-03)

CONVERTER DEW POINT CHECK -

BED TEMPERATURE	DEW POINT TEMPERATURE	TEMPERATURE DIFFERENCE	BED PRESSURE
434.596	397.984	36.612	17.170
444.192	407.363	36.830	17.093
453.789	415.332	38.457	17.017
463.385	422.298	41.087	16.940
472.981	428.506	44.475	16.863

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 78.61

PERCENT OF NON-ELEMENTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 68.89

CONVERTER EXIT STREAM -
STREAM NUMBER 16

TEMPERATURE (DEG. F) = 473.0 PRESSURE (PSIA) = 16.86
STREAM ENTHALPY (BTU.) = -0.5042203E 08

MOLE NUMBERS ARE -

CH4 -	0.00000	CO2 -	105.85832
O2 -	0.00000	N2 -	557.29297
H2O -	340.24756	H2S -	7.34552
SO2 -	3.65896	S -	0.0
S2 -	0.01233	S6 -	1.88656
S8 -	3.63693	COS -	0.00086
CS2 -	0.00000	H2 -	0.00073
CO -	0.00000	S -	0.0

CONDENSER 3
EQUIPMENT NUMBER 11

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 473.0 PRESSURE (PSIA) = 16.86
STEAM ENTHALPY (BTU.) = -0.5042203E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	105.85832
O2	-	0.00000	N2	-	557.29297
H2O	-	340.24756	H2S	-	7.34552
SO2	-	3.65896	S	-	0.0
S2	-	0.01233	S6	-	1.88656
S8	-	3.63693	COS	-	0.00086
CS2	-	0.00000	H2	-	0.00073
CO	-	0.00000	S	-	0.0

CONDENSER DESIGN

TUBE LENGTH (FT.) = 13.3
TUBE DIAMETER (IN.) = 1.000
NUMBER OF TUBES = 359

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.00
OUTLET GAS TEMPERATURE (DEG.F) = 308.9
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 14.39

EQUIP. HEAT DUTY (BTU/HR) IS 0.1525291E 07

STEAM TEMP. (DEG.F) = 281.1
PRESS. (PSIA) = 50.000
LATENT HEAT (BTU/LB) = 924.7
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.1649466E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 94.66, PERCENT RECOVERY = 37.06

SULPHUR FOG - 23.29 MOLES, OR 745.3 LBS.
SULPHUR LIQUID - 14.99 MOLES, OR 479.6 LBS.
(STREAM NO. 18 , TEMPERATURE = 285.3 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 4.00

EXISTENCE OF COALESCER IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 94.66, PERCENT RECOVERY = 91.52

SULPHUR FOG - 1.27 MOLES, OR 40.6 LBS.
SULPHUR LIQUID - 37.01 MOLES, OR 1184.3 LBS.
(STREAM NO. 13 , TEMPERATURE = 299.4 DEG.F.)

CONDENSER GASFOUS EXIT STPEAM
STREAM NUMBER 17

TEMPERATURE (DEG. F) = 308.9 PRESSURE (PSIA) = 16.70
STREAM ENTHALPY (BTU.) = -0.5203296E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	105.85832
O2	-	0.00000	N2	-	557.29297
H2O	-	340.24756	H2S	-	7.34552
SO2	-	3.65896	S	-	0.0
S2	-	0.00004	S6	-	0.05018
S8	-	0.23244	COS	-	0.00086
CS2	-	0.00000	H2	-	0.00073
CO	-	0.00000	S	-	1.26801

STREAM COMBINER / DIVIDER
EQUIPMENT NUMBER 14

COMBINE STREAMS 9 & 13 & 18

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 322.6 PRESSURE (PSIA) = 16.70
STREAM ENTHALPY (BTU.) = 0.6868596F 06

MOLE NUMBERS ARE -

CH4	-	0.0	CO2	-	0.0
O2	-	0.0	N2	-	0.0
H2O	-	0.0	H2S	-	0.0
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	CDS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	275.60474

EXHAUST GAS INCINERATOR
EQUIPMENT NUMBER 12

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 308.9 PRESSURE (PSIA) = 16.70
STREAM ENTHALPY (BTU.) = -0.5203296E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	105.85832
O2	-	0.00000	N2	-	557.29297
H2O	-	340.24756	H2S	-	7.34552
SO2	-	3.65896	S	-	0.0
S2	-	0.00004	S6	-	0.05018
S8	-	0.23244	COS	-	0.00086
CS2	-	0.00000	H2	-	0.00073
CO	-	0.00000	S	-	1.26801

COMBUSTION AIR -

TEMPERATURE (DEG. F) = 80.0
PRESSURE (PSIA.) = 15.00
RELATIVE HUMIDITY (PERCENT) = 55.00

RATIO (SPECIFIED/STOICHIOMETRIC) AIR ADDED -

FOR COMBUSTION OF PROCESS GAS - 1.250
FOR COMBUSTION OF FUEL GAS - 1.000

FUEL AND AIR STREAM
STREAM NUMBER 19

TEMPERATURE (DEG. F) = 81.7 PRESSURE (PSIA) = 13.00
STREAM ENTHALPY (BTU.) = -0.1535593E 07

MOLE NUMBERS ARE -

CH4	-	27.10800	CO2	-	0.0
O2	-	72.27661	N2	-	271.89746
H2O	-	6.49273	H2S	-	0.0
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	0.0

INCINERATOR EXHAUST STREAM
STREAM NUMBER 20

TEMPERATURE (DEG. F) = 1250.0 PRESSURE (PSIA) = 16.70
STREAM ENTHALPY (BTU.) = -0.5356848E 08

MOLE NUMBERS ARE -

CH4	-	0.0	CO2	-	132.96718
O2	-	3.61202	N2	-	829.19043
H2O	-	408.30200	H2S	-	0.0
SO2	-	14.43400	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.00000
CO	-	0.00000	S	-	0.0

SULPHUR PLANT STACK
EQUIPMENT NUMBER 13

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 1250.0 PRESSURE (PSIA) = 16.70
STREAM ENTHALPY (BTU.) = -0.5356848E 08

MOLE NUMBERS ARE -

CH4	-	0.0	CO2	-	132.96718
O2	-	3.61202	N2	-	829.19043
H2O	-	408.30200	H2S	-	0.0
SO2	-	14.43400	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.00000
CO	-	0.00000	S	-	0.0

SULPHUR PLANT STACK DESIGN

AMBIENT TEMPERATURE (DEG.F) = 75.0
EQUIVALENT STACK TEMPERATURE (DEG.F) = 69.8
TOTAL GASEOUS STACK FLOWRATE (C.F.S. AT TEQIV) = 131.3
POLLUTANT (SO2) FLOWRATE (C.F.S. AT TEQIV) = 1.365
STACK OUTLET TEMPERATURE (DEG.F) = 1175.0

STACK DIAMETER (FT. AT TOP) = 1.45
STACK VELOCITY (FT/SEC. AT TOP) = 80.00

ATMOSPHERIC CONDITIONS

-----	-----
STABLE	UNSTABLE
-----	-----

STACK HEIGHT (FT.) =	135.8	116.1
MAX. GROUND CONCENTRATION (PPM) =	0.2000	0.2000
WIND SPEED AT MAX. (FT/SEC) =	14.67	14.67
DISTANCE (SOURCE TO MAX., FT.) =	4670.	2335.
EFFECTIVE STACK HEIGHT (FT.) =	233.5	233.5

OVERALL PLANT MASS AND ENERGY BALANCE

ATOM AND TOTAL MASS BALANCES

ATOM TYPE	ATOM TOTAL	PERCENT ERROR
S	0.290041E 03	0.00093
O	0.710332E 03	0.00055
C	0.132967E 03	0.00014
H	0.816611E 03	0.00087
N	0.165838E 04	0.00006
TOTAL	0.360833E 04	0.00041

ENERGY BALANCE

(ENTHALPY IS RELATIVE AND IN BTU.)

ENTHALPY IN = -0.274555E 08

ENTHALPY OUT = -0.538001E 08

DIFFERENCE = 0.263445E 08

DIFFERENCE SHOULD BE TOTAL PLANT HEAT LOAD

OVERALL PLANT SULPHUR RECOVERY

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 95.02

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 1

COMBUSTION AIR ADDER

1 = 0.200000E 01 *
3 = 0.750000E 02 *
5 = 0.100000E 01 *

2 = 0.450000E 02 *
4 = 0.185000E 02 *
6 = 0.333300E 00 *

EQUIPMENT NUMBER 2

COMBINER/DIVIDER

1 = 0.305369E-01

2 = 0.500000E 01 *

EQUIPMENT NUMBER 8

IN-LINE BURNER

1 = 0.100000E 02
3 = 0.224476E 01
5 = 0.201018E 04

2 = 0.240000E 02
4 = 0.189452E 05 *

EQUIPMENT NUMBER 3

WASTE HEAT BOILER

1 = 0.300000E 01 *
3 = 0.100000E 01 *
5 = 0.740000E 02
7 = 0.250000E 01 *
9 = 0.167207E 04
11 = 0.599416E 03 *
13 = 0.186333E 00
15 = 0.883833E 00 *
17 = 0.0
19 = 0.123179E 00
21 = 0.0
23 = 0.0
25 = 0.160000E 04 *
27 = 0.250000E 03

2 = 0.200000E 02
4 = 0.890000E 02
6 = 0.600000E 02 *
8 = 0.200000E 01 *
10 = 0.900392E 03 *
12 = 0.287693E-02
14 = 0.369396E 00
16 = 0.481173E 05
18 = 0.0
20 = 0.700000E 01 *
22 = 0.0
24 = 0.0
26 = 0.201019E 04
28 = 0.185544E 08

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 5 CONDENSER

1 =	0.100000E 01 *	2 =	0.107331E 02
3 =	0.100000E 01	4 =	0.387000E 03
5 =	0.500000E 02	6 =	0.400478E 01
7 =	0.900000E 01 *	8 =	0.364891E 03 *
9 =	0.0	10 =	0.250000E 02 *
11 =	0.901139E 02	12 =	0.258371E 07

EQUIPMENT NUMBER 4 ADIABATIC COMBINER

1 =	0.450000E 03 *	2 =	0.450000E 03
3 =	0.700000E 01 *		

EQUIPMENT NUMBER 6 CONVERTER

1 =	0.100000E 01 *	2 =	0.161598E 03
3 =	0.300000E 01	4 =	0.484794E 03
5 =	0.450913E 00	6 =	0.100000E 01
7 =	0.211050E 01	8 =	0.150000E 00 *

EQUIPMENT NUMBER 7 CONDENSER

1 =	0.200000E 01 *	2 =	0.118616E 02
3 =	0.100000E 01	4 =	0.386000E 03
5 =	0.500000E 02	6 =	0.399569E 01
7 =	0.130000E 02 *	8 =	0.347527E 03 *
9 =	0.0	10 =	0.130000E 02 *
11 =	0.903994E 02	12 =	0.275057E 07

EQUIPMENT NUMBER 9 ADIABATIC COMBINER

1 =	0.425000E 03 *	2 =	0.425000E 03
3 =	0.140000E 02 *		

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 10

CONVERTER

1 =	0.200000E 01 *	2 =	0.163043E 03
3 =	0.300000E 01	4 =	0.489129E 03
5 =	0.383130E 00	6 =	0.100000E 01
7 =	0.209567E 01	8 =	0.150000E 00 *

EQUIPMENT NUMBER 11

CONDENSER

1 =	0.300000E 01 *	2 =	0.132723E 02
3 =	0.100000E 01	4 =	0.359000E 03
5 =	0.500000E 02	6 =	0.399556E 01
7 =	0.180000E 02 *	8 =	0.308856E 03 *
9 =	0.0	10 =	0.400000E 01 *
11 =	0.915210E 02	12 =	0.152529E 07

EQUIPMENT NUMBER 14

COMBINER/DIVIDER

1 =	0.0	2 =	0.0
-----	-----	-----	-----

EQUIPMENT NUMBER 12

INCINERATOR

1 =	0.125000E 04 *	2 =	0.550000E 02 *
3 =	0.800000E 02 *	4 =	0.150000E 02 *
5 =	0.125000E 01 *	6 =	0.100000E 01 *
7 =	0.190000E 02 *		

EQUIPMENT NUMBER 13

STACK

1 =	0.750000E 02 *	2 =	0.117500E 04 *
3 =	0.135806E 03	4 =	0.144555E 01
5 =	0.200000E 00 *	6 =	0.800000E 02 *
7 =	0.200000E 02	8 =	0.100000E 01

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE - COMPOSITION - MOLES/HR.
ENTHALPY - MMBTU./HR. VOLUME - CU.FT./MIN. (GAS ONLY)
TEMPERATURE - DEG.F. PRESSURE - PSIA.

STREAM NO.	1	2	3	4	5
CH4	1.5677	0.0	1.5677	1.5198	0.0479
CO2	104.2917	0.0	104.2917	101.1069	3.1847
O2	0.0	148.1414	148.1414	143.6176	4.5238
N2	0.0	557.2935	557.2935	540.2754	17.0180
H2O	47.0000	7.4202	54.4202	52.7584	1.6618
H2S	290.0413	0.0	290.0413	281.1841	8.8570
SO2	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0
S2	0.0	0.0	0.0	0.0	0.0
S6	0.0	0.0	0.0	0.0	0.0
S8	0.0	0.0	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0
CS2	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0
TOT. MOLES	442.900	712.855	1155.755	1120.462	35.293
TOT. LBS.	15321.3	20478.3	35799.6	34706.4	1093.2
TOT.LB.S(M)	0.0	0.0	0.0	0.0	0.0
TOT.LB.S(E)	9281.3	0.0	9281.3	8997.9	283.4
ENTHALPY	-25.138	-0.782	-25.920	-25.128	-0.792
VOLUME	2208.1	3684.5	5950.0	5768.3	181.7
TEMPERATURE	70.00	75.00	72.87	72.87	72.87
S. DEW PT.	0.0	0.0	0.0	0.0	0.0
PRESSURE	19.00	18.50	18.50	18.50	18.50

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE - COMPOSITION - MOLES/HR.
ENTHALPY - MMBTU./HR. VOLUME - CU.FT./MIN. (GAS ONLY)
TEMPERATURE - DEG.F. PRESSURE - PSIA.

STREAM NO.	6	7	8	9	10
CH4	0.0000	0.0000	0.0000	0.0	0.0000
CO2	86.9204	12.2117	86.9204	0.0	99.1321
O2	0.0	0.0	0.0	0.0	0.0
N2	473.7246	66.5507	473.7246	0.0	540.2751
H2O	231.3343	32.4902	231.3343	0.0	263.8245
H2S	58.8436	8.2775	58.8436	0.0	67.1211
SO2	33.5897	4.7227	33.5897	0.0	38.3124
S	0.0	0.0000	0.0	0.0	0.0
S2	0.2508	2.7150	0.0003	0.0	0.0064
S6	10.2668	2.1534	0.2310	0.0	1.4928
S8	11.4034	0.3975	0.8500	0.0	3.4653
COS	0.7410	0.1043	0.7410	0.0	0.8452
CS2	0.0018	0.0003	0.0018	0.0	0.0021
H2	5.2941	0.7412	5.2941	0.0	6.0353
CO	2.3220	0.3252	2.3220	0.0	2.6473
S	0.0	0.0	6.9748	138.2070	0.0
TOT. MOLES	914.696	130.690	900.826	138.207	1023.159
TOT. LBS.	30431.2	4275.1	26008.6	4422.6	30283.7
TOT.LB.S(M)	4907.8	689.0	485.2	4422.6	1174.2
TOT.LB.S(F)	7839.5	1108.3	3466.9	4422.6	4575.2
ENTHALPY	-38.711	-4.965	-41.660	0.356	-46.626
VOLUME	9651.3	1735.8	7388.9	*****	9330.8
TEMPERATURE	599.42	900.39	364.89	331.40	450.00
S. DEW PT.	514.87	551.37	364.69	0.0	425.79
PRESSURE	17.95	18.31	17.84	17.84	17.84

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE - COMPOSITION - MOLES/HR.
ENTHALPY - MMBTU./HR. VOLUME - CU.FT./MIN. (GAS ONLY)
TEMPERATURE - DEG.F. PRESSURE - PSIA.

STREAM NO.	11	12	13	14	15
CH4	0.0000	0.0000	0.0	0.0000	0.0000
CO2	102.6190	102.6190	0.0	2.7781	105.3971
O2	0.0	0.0	0.0	0.0000	0.0000
N2	540.2751	540.2751	0.0	17.0180	557.2930
H2O	315.2825	315.2825	0.0	8.4710	323.7534
H2S	21.6918	21.6918	0.0	1.5139	23.2057
SO2	10.8384	10.8384	0.0	1.2986	12.1370
S	0.0	0.0	0.0	0.0001	0.0
S2	0.3042	0.0002	0.0	3.0069	0.0027
S6	8.2606	0.1604	0.0	0.0000	0.6544
S8	7.5332	0.6328	0.0	0.0	1.5165
COS	0.0076	0.0076	0.0	0.0304	0.0380
CS2	0.0000	0.0000	0.0	0.0001	0.0001
H2	0.0056	0.0056	0.0	0.6296	0.6353
CO	0.0001	0.0001	0.0	0.4240	0.4241
S	0.0	4.0248	100.3872	0.0	0.0
TOT. MOLES	1006.817	995.537	100.387	35.171	1025.056
TOT. LBS.	30233.7	27071.3	3212.4	1093.2	28164.4
TOT.LB.S(M)	3534.0	321.6	3212.4	192.4	514.0
TOT.LB.S(E)	4575.2	1362.8	3212.4	283.4	1646.2
ENTHALPY	-46.626	-49.630	0.247	-0.792	-50.422
VOLUME	11072.7	3299.2	*****	839.7	9403.4
TEMPERATURE	609.62	347.53	318.87	2010.18	425.00
S. DEW PT.	488.06	347.41	0.0	611.26	386.52
PRESSURE	17.39	17.25	17.25	18.50	17.25

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE -

COMPOSITION - MOLES/HR.

ENTHALPY - MMBTU./HR.

VOLUME - CU.FT./MIN. (GAS ONLY)

TEMPERATURE - DEG.F.

PRESSURE - PSIA.

STREAM NO.	16	17	18	19	20
CH4	0.0000	0.0000	0.0	27.1080	0.0
CO2	105.8583	105.8583	0.0	0.0	132.9672
O2	0.0000	0.0000	0.0	72.2766	3.6120
N2	557.2930	557.2930	0.0	271.8975	829.1904
H2O	340.2476	340.2476	0.0	6.4927	408.3020
H2S	7.3455	7.3455	0.0	0.0	0.0
SO2	3.6590	3.6590	0.0	0.0	14.4340
S	0.0	0.0	0.0	0.0	0.0
S2	0.0123	0.0000	0.0	0.0	0.0
S6	1.3866	0.0502	0.0	0.0	0.0
S8	3.6369	0.2324	0.0	0.0	0.0
COS	0.0009	0.0009	0.0	0.0	0.0
CS2	0.0000	0.0000	0.0	0.0	0.0
H2	0.0007	0.0007	0.0	0.0	0.0000
CO	0.0000	0.0000	0.0	0.0	0.0000
S	0.0	1.2680	37.0106	0.0	0.0
TOT. MOLES	1019.940	1015.955	37.011	377.775	1388.505
TOT. LBS.	28164.4	26980.1	1184.3	10476.6	37456.7
TOT.LB.S(M)	1294.1	109.7	1184.3	0.0	0.0
TOT.LB.S(E)	1646.2	461.9	1184.3	0.0	461.9
ENTHALPY	-50.422	-52.033	0.084	-1.536	-53.568
VOLUME	10088.1	8351.6	*****	2813.7	25423.3
TEMPERATURE	472.98	308.86	299.42	81.74	1250.00
S. DEW PT.	428.50	308.82	0.0	0.0	0.0
PRESSURE	16.86	16.70	16.70	13.00	16.70

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE - COMPOSITION - MOLES/HR.
ENTHALPY - MMBTU./HR. VOLUME - CU.FT./MIN. (GAS ONLY)
TEMPERATURE - DEG.F. PRESSURE - PSIA.

STREAM NO.	21	22	30	31	32
CH4	0.0	0.0	0.0	0.0	0.0
CO2	132.9672	0.0	0.0	0.0	0.0
O2	3.6120	0.0	0.0	0.0	0.0
N2	829.1904	0.0	0.0	0.0	0.0
H2O	408.3020	0.0	1253.8987	1253.8987	155.2252
H2S	0.0	0.0	0.0	0.0	0.0
SO2	14.4340	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0
S2	0.0	0.0	0.0	0.0	0.0
S6	0.0	0.0	0.0	0.0	0.0
S8	0.0	0.0	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0
CS2	0.0	0.0	0.0	0.0	0.0
H2	0.0000	0.0	0.0	0.0	0.0
CO	0.0000	0.0	0.0	0.0	0.0
S	0.0	275.6047	0.0	0.0	0.0
TOT. MOLFS	1388.505	275.605	1253.899	1253.899	155.225
TOT. LBS.	37456.7	8819.4	22570.2	22570.2	2794.1
TOT.LB.S(M)	0.0	8819.4	0.0	0.0	0.0
TOT.LB.S(F)	461.9	8819.4	0.0	0.0	0.0
ENTHALPY	-54.487	0.687	*****	*****	*****
VOLUME	24308.0	*****	*****	*****	*****
TEMPERATURE	1175.00	322.59	400.99	400.99	281.05
S. DEW PT.	0.0	0.0	0.0	0.0	0.0
PRESSURE	16.70	16.70	250.00	250.00	50.00

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE -

COMPOSITION - MOLES/HR.

ENTHALPY - MMBTU./HR.

VOLUME - CU.FT./MIN. (GAS ONLY)

TEMPERATURE - DEG.F.

PRESSURE - PSIA.

STREAM NO.	33	34	35	36	37
CH4	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	0.0
H2O	155.2252	165.2498	165.2498	91.6370	91.6370
H2S	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0
S2	0.0	0.0	0.0	0.0	0.0
S6	0.0	0.0	0.0	0.0	0.0
S8	0.0	0.0	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0
CS2	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0
TOT. MOLES	155.225	165.250	165.250	91.637	91.637
TOT. LBS.	2794.1	2974.5	2974.5	1649.5	1649.5
TOT.LB.S(M)	0.0	0.0	0.0	0.0	0.0
TOT.LB.S(E)	0.0	0.0	0.0	0.0	0.0
ENTHALPY	*****	*****	*****	*****	*****
VOLUME	*****	*****	*****	*****	*****
TEMPERATURE	281.05	281.05	281.05	281.05	281.05
S. DEW PT.	0.0	0.0	0.0	0.0	0.0
PRESSURE	50.00	50.00	50.00	50.00	50.00

EXAMPLE 2.

SPECIFICATIONS

PLANT FEED ACID GAS, MOLES/HR.

CH ₄	10.57
CO ₂	109.41
H ₂ O	63.67
H ₂ S	965.65

COMBUSTION AIR

PERCENT OF STOICHIOMETRIC
REQUIREMENTS

HYDROGEN SULPHIDE FEED

33.3

SPECIFIED TEMPERATURES AND PRESSURES

DEG.F.

PSIA.

ACID GAS FEED

110.

18.4

PRIMARY COMBUSTION AIR (R.H. = 5.72)

191.

20.

INCINERATOR FUEL GAS (METHANE)

100.

13.

BOILER BYPASS

1200.

BOILER EXIT

550.

BOILER STEAM

313.

PRIMARY (BOILER) EQUILIBRIUM CUTOFF

1800.

NO. 1. CONVERTER INLET

455.

NO. 2. CONVERTER INLET

400.

14.5

NO. 1 CONDENSER EXIT

375.

NO. 2. CONDENSER INLET

525.

15.9

NO. 2 CONDENSER EXIT

335.

NO. 3 CONDENSER EXIT

265.

FIRST AND SECOND CONDENSER STEAM

78.

THIRD CONDENSER STEAM

33.

INCINERATOR PROCESS EXIT

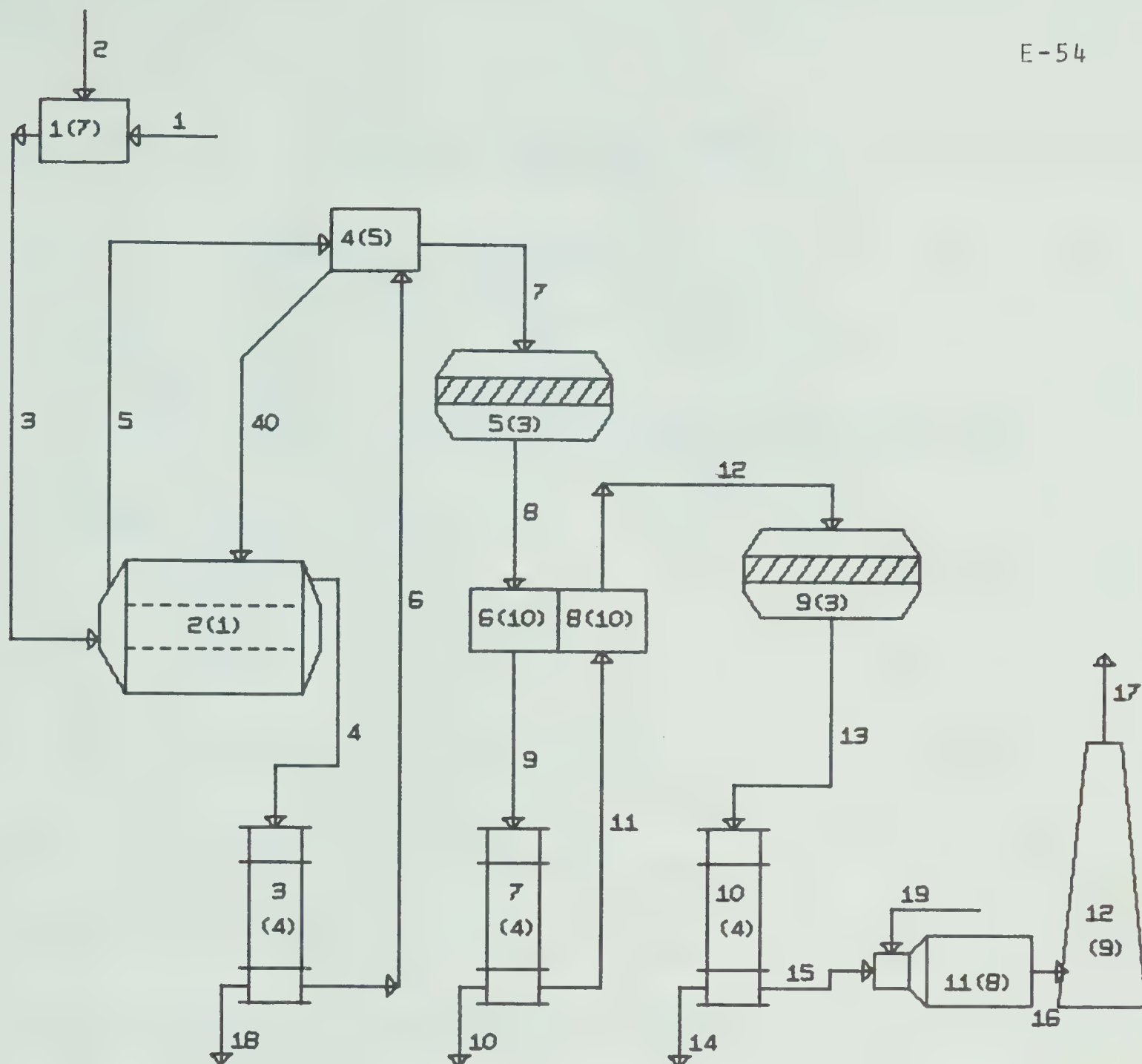
1100.

STACK EXIT

900.

MISCELLANEOUS

- 2 PASS BOILER 24 FT. LONG
- MAXIMUM ALLOWABLE PRESSURE DROPS IN 2ND AND 3RD BOILER PASSES 0.6 AND 1.2 PSIA RESPECTIVELY.
- MIN. FLAME REACTION RESIDENCE TIME 0.6 SEC.
- AVERAGE CATALYST PARTICLE SIZE 0.20 IN.
- MAXIMUM ALLOWABLE FOG IN 1ST, 2ND, AND 3RD CONDENSERS 5, 3, AND 1 LB.(S)/100 MOLES INERT EXIT GAS RESPECTIVELY



LEGEND

NUMBERS DENOTE STREAM OR EQUIPMENT NUMBERS

NUMBERS IN BRACKETS DENOTE EQUIPMENT TYPES -

- | | |
|------------------------|---------------------|
| 1. WASTE HEAT BOILER | 6. COMBINER/DIVIDER |
| 2. INLINE BURNER | 7. AIR ADDER |
| 3. CATALYTIC CONVERTER | 8. INCINERATOR |
| 4. SULPHUR CONDENSER | 9. EFFLUENT STACK |
| 5. ADIABATIC COMBINER | 10. BLACK BOX |

FIG. E-2 EQUIPMENT MODULE (PROCESS)
FLOWSHEET FOR EXAMPLE 2.

PROGRAM DATA (CARD IMAGE)

C EXAMPLE 2. (DESIGN)

PROGRAM CONTROL PARAMETERS

1 1 1 1 1 1 1 1 1 1 0 0 0 0 0

END

FLOWSHEET DATA

1 0 1**2 0 1**3 1 2**4 2 3**5 2 4**6 3 4**7 4 5**8 5 6**

9 6 7**10 7 0**11 7 8**12 8 9**13 9 10**14 10 0**15 10 11**

16 11 12**17 12 0**18 3 0**19 0 11**40 4 2 1 -1**

END

STREAM SPECIFICATIONS

1 1 10.57 2 109.41 5 63.67 6 965.65 21 110. 22 18.4**

9 21 525. 22 15.9**

12 21 400. 22 14.5**

19 1 20. 21 100. 22 13.**

40 1 19.**

END

EQUIPMENT PARAMETER SPECIFICATIONS

1 7,2 1,3 4,4 5,5 3,6 10,7 4,8 10,9 3,10 4,11 8,12 9**

1 1 2. 2 5.72 3 191. 4 20. 6 0.33333**

2 1 2. 2 24. 9 1200. 10 550. 12 .6 13 1.2 15 .6 19 .1

20 5. 25 1800. 27 313. **

3 1 1. 5 78. 7 18. 8 375. 10 5.**

4 1 455. 3 5.**

5 1 1. 8 .2 **

7 1 2. 5 78. 7 10. 8 335. 10 3.**

9 1 2. 8 .2 **

10 1 3. 5 33. 7 14. 8 265. 10 1.**

11 1 1100. 7 19.**

12 2 900.**

END

*MOLECULAR AND THERMODYNAMIC DATA***

'H' 1.,3.7 'C' 12.,14.8 'O' 16.,7.4 'S' 32.,25.6

'N' 14. 15.6 **

'CH4 '

+4.2497678E+00 -6.9126562E-03 +3.1602134E-05 -2.9715432E-08

+9.5103580E-12 -1.0186632E+04 -9.1754991E-01

+1.1795744E+00 +1.0950594E-02 -4.0622131E-06 +7.1370281E-10

-4.7490353E-14 -9.8556627E+03 +1.2505934E+01 **

'CO2 ', 0.0135, 0.0000205

+2.1701000E+00 +1.0378115E-02 -1.0733938E-05 +6.3459175E-09

-1.6280701E-12 -4.8352602E+04 +1.0664388E+01

+4.4129266E+00 +3.1922896E-03 -1.2978230E-06 +2.4147446E-10

-1.6742986E-14 -4.8944043E+04 -7.2875769E-01 **

'O2 G' 0.02, 0.00002

+3.7139946E+00 -2.5167288E-03 +8.5837353E-06 -8.2998716E-09

+2.7032180E-12 -1.0576706E+03 +3.9080704E+00

+3.5976129E+00 +7.8145603E-04 -2.2386670E-07 +4.2490159E-11

-3.3460204E-15 -1.1927918E+03 +3.7492659E+00 **

PROGRAM DATA (CARD IMAGE)

'N2 ' , 'G', 0.0175 , 0.0000195

+3.6916148E+00 -1.3332552E-03 +2.6503100E-06 -9.7688341E-10
 -9.9772234E-14 -1.0628336E+03 +2.2874980E+00
 +2.8545761E+00 +1.5976316E-03 -6.2566254E-07 +1.1315849E-10
 -7.6897070E-15 -8.9017445E+02 +6.3902879E+00 **

'H2O ' , 'G', 0.008, 0.000021

+4.1565016E+00 -1.7244334E-03 +5.6982316E-06 -4.5930044E-09
 +1.4233654E-12 -3.0288770E+04 -6.8616246E-01
 +2.6707532E+00 +3.0317115E-03 -8.5351570E-07 +1.1790853E-10
 -6.1973568E-15 -2.9883994E+04 +6.8838391E+00 **

'H2S ' , 'G', 0.011 0.000024

+3.9163074E+00 -3.5138671E-04 +4.2191312E-06 -2.7453665E-09
 +4.8534365E-13 -3.6095585E+03 +2.3660042E+00
 +2.7657149E+00 +4.0131914E-03 -1.5044898E-06 +2.6807998E-10
 -1.7967681E-14 -3.3859808E+03 +7.9327186E+00 **

'SO2 ' , 'G' .0115 .000017

+3.2257132E+00 +5.6551207E-03 -2.4970208E-07 -4.2206766E-09
 +2.1392733E-12 -3.6904476E+04 +9.8177036E+00
 +5.1982451E+00 +2.0595095E-03 -8.6254450E-07 +1.6636523E-10
 -1.1847837E-14 -3.7541457E+04 -8.3059963E-01 **

'S ' , 'G'

+2.9137253E+00 +3.1294061E-04 -2.6092508E-06 +3.1382439E-09
 -1.1708988E-12 +3.2568272E+04 +3.5681154E+00
 +2.9145770E+00 -5.6619390E-04 +2.8497584E-07 -5.1868520E-11
 +3.2709932E-15 +3.2604940E+04 +3.7640850E+00 **

'S2 ' , 'G'

+2.6999349E+00 +6.2749549E-03 -9.2370775E-06 +6.5393276E-09
 -1.7802282E-12 +1.4504935E+04 +1.0534222E+01
 +4.1896932E+00 +3.8469704E-04 -1.5566633E-07 +3.0368010E-11
 -2.1795849E-15 +1.4188133E+04 +3.2930300E+00 **

'S6 ' , 'G'

+6.0892429E+00 +1.8824865E-02 -2.7861233E-05 +1.9617983E-08
 -5.3406846E-12 +1.1264370E+04 +7.3202322E+00
 +1.0558515E+01 +1.1540911E-03 -4.6699899E-07 +9.1104030E-11
 -6.5337547E-15 +1.0313964E+04 -1.4403344E+01 **

'S8 ' , 'G'

+7.7838968E+00 +2.5099820E-02 -3.7148310E-05 +2.6157310E-08
 -7.1209128E-12 +1.0114584E+04 +4.7621792E+00
 +1.3742926E+01 +1.5387882E-03 -6.2266532E-07 +1.2147204E-10
 -3.7183396E-15 +8.8473760E+03 -2.4202589E+01 **

'S L'

-4.1562591E+01 +2.8300951E-01 -6.2124646E-04 +5.7917986E-07
 -1.9550879E-10 +4.4720883E+03 1.7978686E+02 3.8716625
 0. 0. 0. 0. -8.4632533E+02 -1.7492768E+01 **

END OF ALL DATA

SULPHUR PLANT DESIGN AND SIMULATION

PROGRAM CONTROL PARAMETERS

END

FLOWSHEET DATA

END

STREAM SPECIFICATIONS

END

EQUIPMENT PARAMETER SPECIFICATIONS

END

MOLECULAR AND THERMODYNAMIC DATA

END OF ALL DATA

CALCULATION SEQUENCE OPTIMIZATION

INITIAL SEQUENCE IS -

1 2 3 4 5 6 7 8 9 10 11 12

THE OPTIMIZED CALCULATION SEQUENCE IS -

1 2 3 4 5 6 7 8 9 10 11 12

THE FOLLOWING STREAMS MUST BE ASSUMED,

40

PRIMARY REACTION CUT-OFF TEMPERATURE (BOILER) = 1800. DEG.F

COMBUSTION AIR ADDER
EQUIPMENT NUMBER 1

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 110.0 PRESSURE (PSIA) = 18.40
STREAM ENTHALPY (BTU.) = -0.3355048E 08

MOLE NUMBERS ARE -

CH4	-	10.57000	CO2	-	109.40999
O2	-	0.0	N2	-	0.0
H2O	-	63.66998	H2S	-	965.64966
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	S	-	0.0

TOTAL MOLES AIR ADDED = 2467.06 (R.H. = 5.72 PERCENT)
MOLES DRY AIR = 2399.81 MOLES WATER = 67.25
TEMPERATURE (DEG.F.) = 191.0 PRESSURE (PSIA.) = 20.00

RATIO OF (SPECIFIED/STOICHIOMETRIC) AIR ADDED -

- FOR OXIDATION OF SULPHUR (ALL H2S) - 0.3333
- FOR OXIDATION OF CARBON, HYDROGEN AND ABOVE - 1.0000

COMBINED OUTLET STREAM
STREAM NUMBER 3

TEMPERATURE (DEG. F) = 162.1 PRESSURE (PSIA) = 18.40
STREAM ENTHALPY (BTU.) = -0.3857349E 08

MOLE NUMBERS ARE -

CH4	-	10.57000	CO2	-	109.40999
O2	-	503.95972	N2	-	1895.84839
H2O	-	130.92152	H2S	-	965.64966
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	S	-	0.0

COMBUSTION REACTION AND WASTE HEAT BOILER.
EQUIPMENT NUMBER 2

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 162.1 PRESSURE (PSIA) = 18.40
STREAM ENTHALPY (BTU.) = -0.3857349E 08

MOLE NUMBERS ARE -

CH4	-	10.57000	CO2	-	109.40999
O2	-	503.95972	N2	-	1895.84839
H2O	-	130.92152	H2S	-	965.64966
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	S	-	0.0

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 2414.9 DEG. F
PRESSURE (PSIA.) = 18.40 (CRIT = 0.10E-03)

STREAM ENTHALPY (BTU.) = -0.3857352E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97997
O2	-	0.00000	N2	-	1895.84839
H2O	-	941.37744	H2S	-	176.33324
SO2	-	88.16147	S	-	0.11131
S2	-	350.52124	S6	-	0.00000
S8	-	0.0	S	-	0.0

MUFFLE FURNACE - (DESIGN)

DIAMETER (IN.) = 72.0 RESIDENCE TIME (SEC.) = 0.510
LENGTH (FT.) = 30.0 HEAT RELEASE (BTU/CU.FT.) = 83348.

DESIGN OF PASS NO. 1

ITERATIVE CALCULATION OF TUBE-PASS TUBE-NUMBER
DELTP SPECIFIED, TDIAM CALCULATED.

CONVERGED TUBE NUMBER IS 104.
TUBE DIAMETER (IN) IS 4.00
TUBE LENGTH (FT) IS 24.00

APPROX. PRESS. DROP (PSI.) = 0.23
APPROX. TOTAL HEAT LOSS (BTU.) = 0.4106085E 08
(ENTH. ERRDR (BTU.) = 0.7408000E 04)

REVERT TO SIMULATION FOR EXACT CALCULATION
OF ACTUAL OUTLET TEMP. AND PRESS. DROP

SIMULATION OF TUBE PASS NO. 1

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 1200.8 DEG. F
PRESSURE (PSIA.) = 18.17 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 4.00
NUMBER OF TUBES = 104.
TUBE LENGTH (FT.) = 24.00
PRESSURE DROP (PSI) = 0.23
TOTAL HEAT LOSS (BTU.) = 0.4102734E 08

STREAM ENTHALPY (BTU.) = -0.7960805E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97997
O2	-	0.0	N2	-	1895.84839
H2O	-	899.72437	H2S	-	217.98630
SO2	-	108.98799	S	-	0.00000
S2	-	315.23657	S6	-	1.33953
S8	-	0.02026	S	-	0.0

BOILER BY-PASS NO. 1 , (RATIO = 0.1000)
STREAM NUMBER 5

TEMPERATURE (DEG. F) = 1200.8 PRESSURE (PSIA) = 18.17
STREAM ENTHALPY (BTU.) = -0.7960707E 07

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	11.99799
O2	-	0.0	N2	-	189.58476
H2O	-	89.97240	H2S	-	21.79861
SO2	-	10.89880	S	-	0.00000
S2	-	31.52364	S6	-	0.13395
S8	-	0.00203	S	-	0.0

DESIGN OF PASS NO. 2

ITERATIVE CALCULATION OF TUBE-PASS TUBE-NUMBER
DELTP SPECIFIED, TDIAM CALCULATED.

CONVERGED TUBE NUMBER IS 1905.
TUBE DIAMETER (IN) IS 1.50
TUBE LENGTH (FT) IS 24.00

APPROX. PRESS. DROP (PSI.) = 0.04
APPROX. TOTAL HEAT LOSS (BTU.) = 0.2972165E 08
(ENTH. ERROR (BTU.) = 0.2016000E 04)

REVERT TO SIMULATION FOR EXACT CALCULATION
OF ACTUAL OUTLET TEMP. AND PRESS. DROP

SIMULATION OF TUBE PASS NO. 2

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 550.0 DEG. F
PRESSURE (PSIA.) = 18.13 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 1.50
NUMBER OF TUBES = 1905.
TUBE LENGTH (FT.) = 24.00
PRESSURE DROP (PSI) = 0.04
TOTAL HEAT LOSS (BTU.) = 0.2972304E 08

BOILER EXIT STREAM -
STREAM NUMBER 4

TEMPERATURE (DEG. F) = 550.0 PRESSURE (PSIA) = 18.13
STREAM ENTHALPY (BTU.) = -0.1013698E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	107.98196
O2	-	0.00000	N2	-	1706.26343
H2O	-	810.04395	H2S	-	195.89563
SO2	-	97.94318	S	-	0.0
S2	-	0.31145	S6	-	30.04912
S8	-	49.29054	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 522.2
STREAM WATER DEW PT. (DEG. F) = 161.4

EQUIP. HEAT DUTY (BTU/HR) IS 0.7075098E 08

STEAM TEMP. (DEG. F.) = 421.3
PRESS. (PSIA) = 313.000
LATENT HEAT (BTU/LB) = 802.2
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.8819188E 05

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 66.18

CONDENSER 1
EQUIPMENT NUMBER 3

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 550.C PRESSURE (PSIA) = 18.13
STREAM ENTHALPY (BTU.) = -0.1013678E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	107.98196
O2	-	0.00000	N2	-	1706.26343
H2O	-	810.04395	H2S	-	195.89563
SO2	-	97.94318	S	-	0.0
S2	-	0.31145	S6	-	30.04912
S8	-	49.29054	S	-	0.0

CONDENSER DESIGN

TUBE LENGTH (FT.) = 11.3
TUBE DIAMETER (IN.) = 1.000
NUMBER OF TUBES = 1253

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.00
OUTLET GAS TEMPERATURE (DEG.F) = 375.0
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 14.11

EQUIP. HEAT DUTY (BTU/HR) IS 0.6986898E 07

STEAM TEMP. (DEG.F.) = 310.3
PRESS. (PSIA) = 78.000
LATENT HEAT (BTU/LB) = 901.6
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.7749449E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 94.10, PERCENT RECOVERY = 37.52

SULPHUR FOG - 325.47 MOLES, OR 10415.1 LBS.
SULPHUR LIQUID - 215.81 MOLES, OR 6905.9 LBS.
(STREAM NO. 13 , TEMPERATURE = 312.8 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 5.00

EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 94.10, PERCENT RECOVERY = 93.30

SULPHUR FOG - 4.56 MOLES, OR 145.9 LBS.
SULPHUR LIQUID - 536.72 MOLES, OR 17175.1 LBS.
(STREAM NO. 18 , TEMPERATURE = 353.0 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 6

TEMPERATURE (DEG. F) = 375.0 PRESSURE (PSIA) = 18.02
STREAM ENTHALPY (BTU.) = -0.1098730E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	107.98196
O2	-	0.00000	N2	-	1706.26343
H2O	-	810.04395	H2S	-	195.89563
SO2	-	97.94318	S	-	0.0
S2	-	0.00156	S6	-	0.99092
S8	-	3.50132	S	-	4.55957

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 4

COMBINE STREAMS 5 AND 6

FIND GIVEN FEED STREAM RESULTANT TEMPERATURE
ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 519.9 DEG. F
PRESSURE (PSIA.) = 18.02 (CRIT = 0.10E-03)

PREDICTED STREAM SPLIT FOR TEMP. OF 455.0000 IS 0.0547
USE STREAMS RESULTING FROM THIS PREDICTION
FOR PRESENT EQUIPMENT OUTLET STREAM.

COMBINED OUTLET STREAM (SULPHUR SHIFT DONE) -
STREAM NUMBER 7

TEMPERATURE (DEG. F) = 455.0 PRESSURE (PSIA) = 18.02
STREAM ENTHALPY (BTU.) = -0.1197563E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97993
O2	-	0.00000	N2	-	1895.84790
H2O	-	900.03076	H2S	-	217.67953
SO2	-	108.83461	S	-	0.0
S2	-	0.02050	S6	-	3.44575
S8	-	6.83768	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 406.2
STREAM WATER DEW PT. (DEG. F) = 162.2

CALCULATIONS LOOPED ON RECYCLE LOOP -

COMBUSTION REACTION AND WASTE HEAT BOILER.
EQUIPMENT NUMBER 2

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 162.1 PRESSURE (PSIA) = 18.40
STREAM ENTHALPY (BTU.) = -0.3857349E 08

MOLE NUMBERS ARE -

CH4	-	10.57000	CO2	-	109.40999
O2	-	503.95972	N2	-	1895.84839
H2O	-	130.92152	H2S	-	965.64966
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	S	-	0.0

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 2414.9 DEG. F
PRESSURE (PSIA.) = 18.40 (CRIT = 0.10E-03)

STREAM ENTHALPY (BTU.) = -0.3857354E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84839
H2O	-	941.37695	H2S	-	176.33365
SO2	-	88.16170	S	-	0.11131
S2	-	350.52075	S6	-	0.00000
S8	-	0.0	S	-	0.0

MUFFLE FURNACE - (DESIGN)

DIAMETER (IN.) = 72.0 RESIDENCE TIME (SEC.) = 0.510
LENGTH (FT.) = 30.0 HEAT RELEASE (BTU/CU.FT.) = 83348.

DESIGN OF PASS NO. 1

ITERATIVE CALCULATION OF TUBE-PASS TUBE-NUMBER
TDIAM SPECIFIED, DELPC CALCULATED.

CONVERGED TUBE NUMBER IS 104.

TUBE DIAMETER (IN) IS 4.00

TUBE LENGTH (FT) IS 24.00

APPROX. PRESS. DROP (PSI.) = 0.23

APPROX. TOTAL HEAT LOSS (BTU.) = 0.4104162E 08

(ENTH. ERROR (BTU.) = -0.2080000E 03)

REVERT TO SIMULATION FOR EXACT CALCULATION
OF ACTUAL OUTLET TEMP. AND PRESS. DROP

SIMULATION OF TUBE PASS NO. 1

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 1200.8 DEG. F
PRESSURE (PSIA.) = 18.17 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 4.00

NUMBER OF TUBES = 104.

TUBE LENGTH (FT.) = 24.00

PRESSURE DROP (PSI) = 0.23

TOTAL HEAT LOSS (BTU.) = 0.4102818E 08

STREAM ENTHALPY (BTU.) = -0.7960774E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.0	N2	-	1895.84839
H2O	-	899.72412	H2S	-	217.98624
SO2	-	108.98799	S	-	0.00000
S2	-	315.23682	S6	-	1.33931
S8	-	0.02025	S	-	0.0

BOILER BY-PASS NO. 1 , (RATIO = 0.0547)
STREAM NUMBER 5

TEMPERATURE (DEG. F) = 1200.8 PRESSURE (PSIA) = 18.17
STREAM ENTHALPY (BTU.) = -0.4357758E 07

MOLF NUMBERS ARE -

CH4	-	0.00000	CO2	-	6.56775
O2	-	0.0	N2	-	103.77948
H2O	-	49.25124	H2S	-	11.93265
SO2	-	5.96604	S	-	0.00000
S2	-	17.25618	S6	-	0.07331
S8	-	0.00111	S	-	0.0

DESIGN OF PASS NO. 2

ITERATIVE CALCULATION OF TUBE-PASS TUBE-NUMBER
TDIAM SPECIFIED, DELPC CALCULATED.

CONVERGED TUBE NUMBER IS 2000.
TUBE DIAMETER (IN) IS 1.50
TUBE LENGTH (FT) IS 24.00

APPROX. PRESS. DROP (PSI.) = 0.04
APPROX. TOTAL HEAT LOSS (BTU.) = 0.3121630E 08
(ENTH. ERROR (BTU.) = 0.1472000E 04)

REVERT TO SIMULATION FOR EXACT CALCULATION
OF ACTUAL OUTLET TEMP. AND PRESS. DROP

SIMULATION OF TUBE PASS NO. 2

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 550.1 DEG. F
PRESSURE (PSIA.) = 18.13 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 1.50
NUMBER OF TUBES = 2000.
TUBE LENGTH (FT.) = 24.00
PRESSURE DROP (PSI) = 0.04
TOTAL HEAT LOSS (BTU.) = 0.3121725E 08

BOILER EXIT STREAM -
STREAM NUMBER 4

TEMPERATURE (DEG. F) = 550.1 PRESSURE (PSIA) = 13.13
STREAM ENTHALPY (BTU.) = -0.1064668E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	113.41223
O2	-	0.00000	N2	-	1792.06885
H2O	-	850.77930	H2S	-	205.74672
SO2	-	102.86850	S	-	0.0
S2	-	0.32727	S6	-	31.56441
S8	-	51.76605	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 522.2
STREAM WATER DEW PT. (DEG. F) = 161.4

EQUIP. HEAT DUTY (BTU/HR) IS 0.7224542E 08

STEAM TEMP. (DEG. F.) = 421.3
PRESS. (PSIA) = 313.000
LATENT HEAT (BTU/LB) = 802.2
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.9005469E 05

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 66.19

CONDENSER 1
EQUIPMENT NUMBER 3

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 550.1 PRESSURE (PSIA) = 18.13
STREAM ENTHALPY (BTU.) = -0.1064668E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	113.41223
O2	-	0.00000	N2	-	1792.06885
H2O	-	850.77930	H2S	-	205.74672
SO2	-	102.86850	S	-	0.0
S2	-	0.32727	S6	-	31.56441
S8	-	51.76605	S	-	0.0

CONDENSER DESIGN

TUBE LENGTH (FT.) = 11.3
TUBE DIAMETER (IN.) = 1.000
NUMBER OF TUBES = 1316

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.00
OUTLET GAS TEMPERATURE (DEG.F) = 375.0
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 14.11

EQUIP. HEAT DUTY (BTU/HR) IS 0.7339024E 07

STEAM TEMP. (DEG.F.) = 310.3
PRESS. (PSIA) = 78.000
LATENT HEAT (BTU/LB) = 901.6
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.8140008E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 94.10, PERCENT RECOVERY = 37.52

SULPHUR FOG - 341.80 MOLES, OR 10937.6 LBS.

SULPHUR LIQUID - 226.70 MOLES, OR 7254.4 LBS.

(STREAM NO. 18 , TEMPERATURE = 319.8 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 5.00EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 94.10, PERCENT RECOVERY = 93.30

SULPHUR FOG - 4.79 MOLES, OR 153.3 LBS.

SULPHUR LIQUID - 563.71 MOLES, OR 18038.8 LBS.

(STREAM NO. 18 , TEMPERATURE = 353.0 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 6TEMPERATURE (DEG. F) = 375.0 PRESSURE (PSIA) = 18.02
STREAM ENTHALPY (BTU.) = -0.1153984E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	113.41223
O2	-	0.00000	N2	-	1792.06885
H2O	-	850.77930	H2S	-	205.74672
SO2	-	102.86850	S	-	0.0
S2	-	0.00164	S6	-	1.04076
S8	-	3.67744	S	-	4.78906

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 4

COMBINE STREAMS 5 AND 6

FIND GIVEN FEED STREAM RESULTANT TEMPERATURE
ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 455.0 DEG. F
PRESSURE (PSIA.) = 18.02 (CRIT = 0.10E-03)

PREDICTED STREAM SPLIT FOR TEMP. OF 455.0000 IS 0.0547
USE STREAMS RESULTING FROM THIS PREDICTION
FOR PRESENT EQUIPMENT OUTLET STREAM.

COMBINED OUTLET STREAM (SULPHUR SHIFT DONE) -
STREAM NUMBER 7

TEMPERATURE (DEG. F) = 455.0 PRESSURE (PSIA) = 18.02
STREAM ENTHALPY (BTU.) = -0.1197562E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	900.03052	H2S	-	217.67937
SO2	-	108.83453	S	-	0.0
S2	-	0.02053	S6	-	3.44720
S8	-	6.83664	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 406.2
STREAM WATER DEW PT. (DEG. F) = 162.2

CONVERTER 1
EQUIPMENT NUMBER 5

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 455.0 PRESSURE (PSIA) = 18.02
STREAM ENTHALPY (BTU.) = -0.1197562E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	900.03052	H2S	-	217.67937
SO2	-	108.83453	S	-	0.0
S2	-	0.02053	S6	-	3.44720
S8	-	6.83664	S	-	0.0

CONVERTER BED (DESIGN)

CROSSSECTIONAL AREA (SQ.FT) = 511.34
THICKNESS (FT.) = 3.00
VOLUME (CU.FT.) = 1534.03
LINEAR GAS VELOCITY (FT./SEC.) = 1.00
MOLAL FLOW RATE (MOLE/HR.SQ.FT.) = 2.12
AVERAGE PARTICLE DIAMETER (IN.) = 0.20
PRESSURE DROP (PSI.) = 0.307

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 584.3 DEG. F
PRESSURE (PSIA.) = 17.71 (CRIT = 0.10F-03)

CONVERTER DEW POINT CHECK -

BED TEMPERATURE	DEW POINT TEMPERATURE	TEMPERATURE DIFFERENCE	BED PRESSURE
480.863	429.555	51.308	17.955
506.726	446.422	60.304	17.893
532.590	459.921	72.669	17.832
558.453	471.347	87.105	17.770
584.316	481.379	102.937	17.709

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 77.81

PERCENT OF NON-ELEMENTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 72.68

CONVERTER EXIT STREAM -
STREAM NUMBER 8

TEMPERATURE (DEG. F) = 584.3 PRESSURE (PSIA) = 17.71
STREAM ENTHALPY (BTU.) = -0.1197562F 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1058.24731	H2S	-	59.46198
SO2	-	29.72585	S	-	0.0
S2	-	0.56853	S6	-	21.55560
S8	-	22.78401	S	-	0.0

BLACK BOX
EQUIPMENT NUMBER 6

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 584.3 PRESSURE (PSIA) = 17.71
STREAM ENTHALPY (BTU.) = -0.1197562E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1058.24731	H2S	-	59.46198
SO2	-	29.72585	S	-	0.0
S2	-	0.56853	S6	-	21.55560
S8	-	22.78401	S	-	0.0

TEMPERATURE CHANGED FROM 584.3 TO 525.0 DEG.F.

(ENTHALPY DIFFERENCE IS -0.162323E 07 BTU/HR.)

STREAM NUMBER 9

TEMPERATURE (DEG. F) = 525.0 PRESSURE (PSIA) = 15.90
STREAM ENTHALPY (BTU.) = -0.1213795E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1058.24731	H2S	-	59.46198
SO2	-	29.72585	S	-	0.0
S2	-	0.17664	S6	-	16.69316
S8	-	26.52879	S	-	0.0

CONDENSER 2
EQUIPMENT NUMBER 7

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 525.0 PRESSURE (PSIA) = 15.90
STREAM ENTHALPY (BTU.) = -0.1213795E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1058.24731	H2S	-	59.46198
SO2	-	29.72585	S	-	0.0
S2	-	0.17664	S6	-	16.69316
S8	-	26.52879	S	-	0.0

CONDENSER DESIGN

TUBE LENGTH (FT.) = 16.0
TUBE DIAMETER (IN.) = 1.000
NUMBER OF TUBES = 1163

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.00
OUTLET GAS TEMPERATURE (DEG.F) = 335.0
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 14.79

EQUIP. HEAT DUTY (BTU/HR) IS 0.6325072E C7

STEAM TEMP. (DEG.F.) = 310.3
PRESS. (PSIA) = 78.000
LATENT HEAT (BTU/LB) = 901.6
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.7015395E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 95.17, PERCENT RECOVERY = 42.96

SULPHUR FOG - 163.26 MOLES, OR 5224.4 LBS.
SULPHUR LIQUID - 134.37 MOLES, OR 4299.8 LBS.
(STREAM NO. 10 , TEMPERATURE = 314.8 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 3.00

EXISTENCE OF COALESCER IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 95.17, PERCENT RECOVERY = 94.22

SULPHUR FOG - 2.97 MOLES, OR 94.9 LBS.
SULPHUR LIQUID - 294.67 MOLES, OR 9429.3 LBS.
(STREAM NO. 10 , TEMPERATURE = 325.8 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 11

TEMPERATURE (DEG. F) = 335.0 PRESSURE (PSIA) = 15.69
STREAM ENTHALPY (BTU.) = -0.1284636E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1058.24731	H2S	-	59.46198
SO2	-	29.72585	S	-	0.0
S2	-	0.00040	S6	-	0.38528
S8	-	1.59974	S	-	2.96556

BLACK BOX
EQUIPMENT NUMBER 8

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 335.0 PRESSURE (PSIA) = 15.69
STREAM ENTHALPY (BTU.) = -0.1284636E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1058.24731	H2S	-	59.46198
SO2	-	29.72585	S	-	0.0
S2	-	0.00040	S6	-	0.38528
S8	-	1.59974	S	-	2.96556

TEMPERATURE CHANGED FROM 335.0 TO 400.0 DEG.F.
(ENTHALPY DIFFERENCE IS 0.159610E 07 BTU/HR.)

STREAM NUMBER 12

TEMPERATURE (DEG. F) = 400.0 PRESSURE (PSIA) = 14.50
STREAM ENTHALPY (BTU.) = -0.1268675E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1058.24731	H2S	-	59.46198
SO2	-	29.72585	S	-	0.0
S2	-	0.00351	S6	-	0.77929
S8	-	1.67415	S	-	0.0

CONVERTER 2
EQUIPMENT NUMBER 9

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 400.0 PRESSURE (PSIA) = 14.50
STREAM ENTHALPY (BTU.) = -0.1268675E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97398
O2	-	0.00000	N2	-	1895.84814
H2O	-	1058.24731	H2S	-	59.46198
SO2	-	29.72585	S	-	0.0
S2	-	0.00351	S6	-	0.77929
S8	-	1.67415	S	-	0.0

CONVERTER BED (DESIGN)

CROSSECTIONAL AREA (SQ.FT) = 583.75
THICKNESS (FT.) = 3.00
VOLUME (CU.FT.) = 1751.24
LINEAR GAS VELOCITY (FT./SEC.) = 1.00
MOLAL FLOW RATE (MOLE/HR.SQ.FT.) = 1.81
AVERAGE PARTICLE DIAMETER (IN.) = 0.20
PRESSURE DROP (PSI.) = 0.190

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 438.3 DEG. F
PRESSURE (PSIA.) = 14.31 (CRIT = 0.10E-03)

CONVERTER DEW POINT CHECK -

BED TEMPERATURE	DEW POINT TEMPERATURE	TEMPERATURE DIFFERENCE	BED PRESSURE
407.656	359.868	47.788	14.462
415.312	373.696	41.616	14.424
422.968	384.405	38.563	14.386
430.624	393.181	37.443	14.348
438.280	400.676	37.604	14.310

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 76.51

PERCENT OF NON-ELEMENTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 71.75

CONVERTER EXIT STREAM -
STREAM NUMBER 13

TEMPERATURE (DEG. F) = 438.3 PRESSURE (PSIA) = 14.31
STREAM ENTHALPY (BTU.) = -0.1268675E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1100.90796	H2S	-	16.80060
SO2	-	8.39517	S	-	0.0
S2	-	0.01558	S6	-	3.43651
S8	-	7.67722	S	-	0.0

CONDENSER 3
EQUIPMENT NUMBER 10

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 438.3 PRESSURE (PSIA) = 14.31
STREAM ENTHALPY (BTU.) = -0.1268675E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84314
H2O	-	1100.90796	H2S	-	16.80060
SO2	-	8.39517	S	-	0.0
S2	-	0.01558	S6	-	3.43651
S8	-	7.67722	S	-	0.0

CONDENSER DESIGN

TUBE LENGTH (FT.) =	18.8
TUBE DIAMETER (IN.) =	1.000
NUMBER OF TUBES =	1043
MAXIMUM FLOW RATE (LB/SQ.FT.SEC) =	4.00
OUTLET GAS TEMPERATURE (DEG.F) =	265.9
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) =	15.05

EQUIP. HEAT DUTY (BTU/HR) IS	0.4585561E 07
STEAM TEMP. (DEG.F.) =	255.9
PRESS. (PSIA) =	33.000
LATENT HEAT (BTU/LB) =	943.8
L.H. CORRECTION =	0.0
PRODUCTION (LB/HR) =	0.4858680E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 97.56, PERCENT RECOVERY = 34.31

SULPHUR FOG - 51.91 MOLES, OR 1661.2 LBS.
SULPHUR LIQUID - 28.15 MOLES, OR 900.9 LBS.
(STREAM NO. 14 , TEMPERATURE = 258.1 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 1.00

EXISTENCE OF COALESCER IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 97.56, PERCENT RECOVERY = 96.37

SULPHUR FOG - 0.98 MOLES, OR 31.4 LBS.
SULPHUR LIQUID - 79.09 MOLES, OR 2530.8 LBS.
(STREAM NO. 14 , TEMPERATURE = 263.1 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 15

TEMPERATURE (DEG. F) = 265.9 PRESSURE (PSIA) = 14.04
STREAM ENTHALPY (BTU.) = -0.1316107E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1100.90796	H2S	-	16.80060
SO2	-	8.39517	S	-	0.0
S2	-	0.00002	S6	-	0.03952
S8	-	0.22032	S	-	0.98186

EXHAUST GAS INCINERATOR
EQUIPMENT NUMBER 11

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 265.9 PRESSURE (PSIA) = 14.04
STREAM ENTHALPY (BTU.) = -0.1316107E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	119.97998
O2	-	0.00000	N2	-	1895.84814
H2O	-	1100.90796	H2S	-	16.80060
SO2	-	8.39517	S	-	0.0
S2	-	0.00002	S6	-	0.03952
S8	-	0.22032	S	-	0.98186

COMBUSTION AIR -

TEMPERATURE (DEG. F) = 70.0
PRESSURE (PSIA.) = 14.04
RELATIVE HUMIDITY (PERCENT) = 50.00

RATIO (SPECIFIED/STOICHIOMETRIC) AIR ADDED -

FOR COMBUSTION OF PROCESS GAS - 1.250
FOR COMBUSTION OF FUEL GAS - 1.250

FUEL AND AIR STREAM
STREAM NUMBER 19

TEMPERATURE (DEG. F) = 72.4 PRESSURE (PSIA) = 13.00
STREAM ENTHALPY (BTU.) = -0.3886507E 07

MOLE NUMBERS ARE -

CH4	-	74.89682	CO2	-	0.0
O2	-	222.47003	N2	-	836.91089
H2O	-	13.81532	H2S	-	0.0
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	S	-	0.0

INCINERATOR EXHAUST STREAM
STREAM NUMBER 16

TEMPERATURE (DEG. F) = 1100.0 PRESSURE (PSIA) = 14.04
STREAM ENTHALPY (BTU.) = -0.1354969F 09

MOLF NUMBERS ARE -

CH4	-	0.0	CO2	-	194.87679
O2	-	44.49391	N2	-	2732.75903
H2O	-	1281.31689	H2S	-	0.0
SO2	-	28.17735	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	S	-	0.0

SULPHUR PLANT STACK
EQUIPMENT NUMBER 12

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 1100.0 PRESSURE (PSIA) = 14.04
STREAM ENTHALPY (BTU.) = -0.1354969E 09

MOLE NUMBERS ARE -

CH4	-	0.0	CO2	-	194.87679
O2	-	44.49391	N2	-	2732.75903
H2O	-	1231.31689	H2S	-	0.0
SO2	-	28.17735	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	S	-	0.0

SULPHUR PLANT STACK DESIGN

AMBIENT TEMPERATURE (DEG.F) = 70.0
EQUIVALENT STACK TEMPERATURE (DEG.F) = 62.8
TOTAL GASEOUS STACK FLOWRATE (C.F.S. AT TEQIV) = 475.3
POLLUTANT (SO2) FLOWRATE (C.F.S. AT TEQIV) = 3.128
STACK OUTLET TEMPERATURE (DEG.F) = 900.0

STACK DIAMETER (FT. AT TOP) = 3.18
STACK VELOCITY (FT/SEC. AT TOP) = 60.00

ATMOSPHERIC CONDITIONS

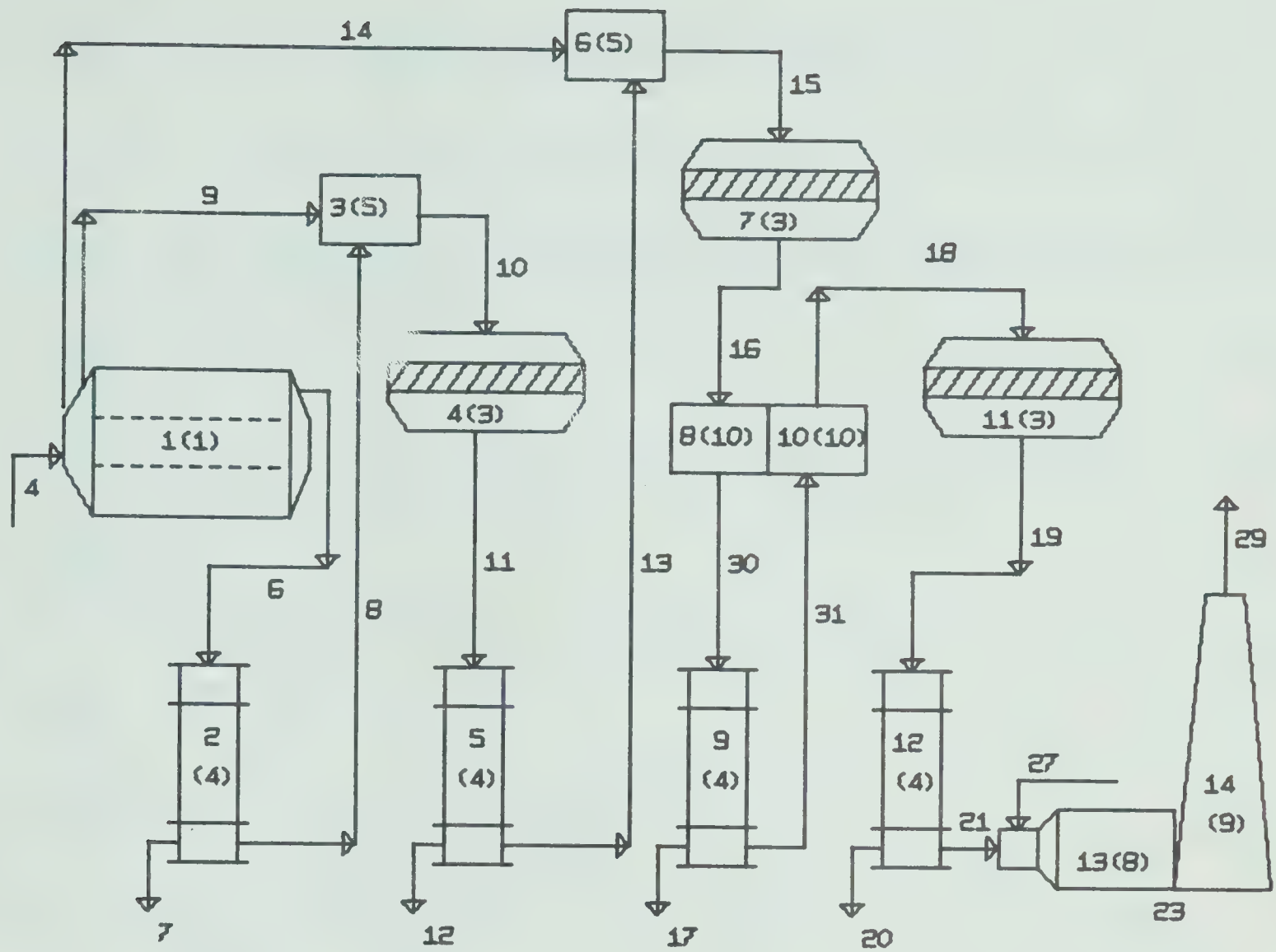
STABLE UNSTABLE

STACK HEIGHT (FT.) =	144.4	116.9
MAX. GROUND CONCENTRATION (PPM) =	0.2000	0.2000
WIND SPEED AT MAX. (FT/SEC) =	14.67	20.00
DISTANCE (SOURCE TO MAX., FT.) =	7070.	2425.
EFFECTIVE STACK HEIGHT (FT.) =	353.5	242.5

EXAMPLE 3.

SPECIFICATIONS

PLANT FEED (MOLES/HR.)	BOILER	INCINERATOR	
CH ₄	3.958	107.62	
CO ₂	310.208		
H ₂ O	163.151	19.87	
H ₂ S	1604.5		
O ₂	761.548	386.64	
N ₂	2864.9	1454.49	
SPECIFIED TEMPERATURES AND PRESSURES		DEG.F.	PSIA.
AMBIENT		80.	
BOILER FEED		127.9	19.1
BOILER STEAM			250.
PRIMARY (BOILER) EQUILIBRIUM CUTOFF		1850.	
SECONDARY (MASKING) CUTOFF		1850.	
NO. 3. CONVERTER INLET		388.	71.2
NO. 2. CONDENSER INLET		383.	17.7
1ST, 2ND, AND 3RD CONDENSER STEAM			68.2
4TH CONDENSER STEAM			30.
INCINERATOR FUEL PLUS AIR		72.	15.
MISCELLANEOUS			
- BOILER	- 3 PASS 27 FT. LONG		
	- FIRST PASS 41 8 IN. TUBES		
	- SECOND PASS 42 8 IN. TUBES		
	- THIRD PASS 1106 1.5 IN. TUBES		
	- MUFFLE FURNACE 72 IN. DIA. X 40 FT. LONG		
	- 1ST AND 2ND BYPASSES .104682 AND .08958 RESP.		
- CONDENSERS	- TUBE DIA. 1.282 IN. FOR ALL FOUR		
	- NUMBER OF TUBES 1025 FOR ALL FOUR		
	- TUBE LENGTHS 20, 20, 16 AND 20 FT. RESP.		
	- MAX. FOG 10, 10, 10, AND 8 LB.(S)/100 MOLES		
	INERT EXIT GAS RESPECTIVELY		
- CONVERTERS	- 1ST, 2ND, AND 3RD CONVERTER CROSS-SECTIONAL		
	AREAS 750, 800, AND 760 SQ.FT. RESPECTIVELY		
	- BED DEPTH 3 FT. FOR ALL THREE		
	- AVERAGE PARTICLE SIZE 0.15 IN.		
- STACK DIA.	3.7 FT. (AT TOP), HEIGHT 130. FT.		



LEGEND

NUMBERS DENOTE STREAM OR EQUIPMENT NUMBERS
NUMBERS IN BRACKETS DENOTE EQUIPMENT TYPES -

- | | |
|------------------------|---------------------|
| 1. WASTE HEAT BOILER | 6. COMBINER/DIVIDER |
| 2. INLINE BURNER | 7. AIR ADDER |
| 3. CATALYTIC CONVERTER | 8. INCINERATOR |
| 4. SULPHUR CONDENSER | 9. EFFLUENT STACK |
| 5. ADIABATIC COMBINER | 10. BLACK BOX |

FIG. E-3 EQUIPMENT MODULE (PROCESS)
FLOWSHEET FOR EXAMPLE 3.

PROGRAM DATA (CARD IMAGE)

```

C          EXAMPLE 3.          (SIMULATION)
C
C          MOLECULAR AND THERMODYNAMIC DATA SAME AS EXAMPLE 1.
C          (TERMINATED BY *END* RATHER THAN *ENDOFALLDATA*)
*PROGRAM CONTROL PARAMETERS*
      1 1 1 1 1 1 1 1 1 1 0 0 0 2 0
*END*
*FLOWSHEET DATA*
      4 0 1**6 1 2**7 2 0**8 2 3**9 1 3**10 3 4**
11 4 5**12 5 0**13 5 6**14 1 6**15 6 7**16 7 8**30 8 9**
31 9 10**17 9 0**18 10 11**19 11 12**20 12 0**21 12 13**
27 0 13**23 13 14**29 14 0**
*END*
*STREAM SPECIFICATIONS*
4      1 3.958 2 310.208 3 761.5476 4 2864.8694 5 163.1511
      6 1604.5      21 127.87      22 19.1      **
30      21 383. 22 17.7**
18      21 388. 22 17.2**
27      1 107.62 3 386.64 4 1454.49 5 19.87 21 72. 22 15. **
*END*
*EQUIPMENT PARAMETER SPECIFICATIONS*
      1 1, 2 4, 3 5, 4 3, 5 4, 6 5, 7 3, 8 10, 9 4, 10 10,
11 3, 12 4, 13 8, 14 9      **
1      1 3. 2 27. 3 41. 4 42. 5 1106. 6 8. 7 8. 8 1.5
      17 40. 18 72. 19 .104682 20 9. 21 .8958E-1 22 14.
      25 1850. 27 250. **
2      1 1. 2 20. 3 1.282 4 1025. 5 68.2 7 7. 10 10.**
5      1 2. 2 20. 3 1.282 4 1025. 5 68.2 7 12. 10 10.**
9      1 3. 2 16. 3 1.282 4 1025. 5 68.2 7 17. 10 10.**
12      1 4. 2 20. 3 1.282 4 1025. 5 30. 7 20. 10 8.**
4      1 1. 2 750. 3 3. 8 0.15 **
7      1 2. 2 800. 3 3. 8 0.15 **
11      1 3. 2 760. 3 3. 8 0.15 **
13      7 27. **
14      1 80. 3 130. 4 3.7 **
*END OF ALL DATA*

```


SULPHUR PLANT DESIGN AND SIMULATION

MOLECULAR AND THERMODYNAMIC DATA

END

PROGRAM CONTROL PARAMETERS

END

FLOWSHEET DATA

ECHO CHECK OF FLOWSHEET DATA

STPFAM NUMBER	SOURCE EQUIP. NO.	DESTINATION EQUIP. NO.	STREAM UNKNOWN	STREAM FLAG
4	0	1	1	0
6	1	2	1	0
7	2	0	1	0
8	2	3	1	0
9	1	3	1	0
10	3	4	1	0
11	4	5	1	0
12	5	0	1	0
13	5	6	1	0
14	1	6	1	0
15	6	7	1	0
16	7	8	1	0
30	8	9	1	0
31	9	10	1	0
17	9	0	1	0
18	10	11	1	0
19	11	12	1	0
20	12	0	1	0
21	12	13	1	0
27	0	13	1	0
23	13	14	1	0
29	14	0	1	0

END

STREAM SPECIFICATIONS

ECHO CHECK OF STREAM SPECIFICATION DATA

STREAM - ' (PARAMETER NO.)PARAMETER VALUE' REPEATED

- 4 - (1) 0.39580E 01 (2) 0.31021E 03 (3) 0.76155E 03
 (4) 0.28649E 04 (5) 0.16315E 03 (6) 0.16045E 04
 (21) 0.12787E 03 (22) 0.19100E 02

- 30 - (21) 0.38300E 03 (22) 0.17700E 02

- 18 - (21) 0.38800E 03 (22) 0.17200E 02

- 27 - (1) 0.10762E 03 (3) 0.38664E 03 (4) 0.14545E 04
 (5) 0.19870E 02 (21) 0.72000E 02 (22) 0.15000E 02

END

EQUIPMENT PARAMETER SPECIFICATIONS

ECHO CHECK OF EQUIPMENT PARAMETER SPECIFICATION DATA

EQUIP. NO.	-	1	2	3	4	5	6	7	8	9	10
		11	12	13	14						
EQUIP. TYPE	-	1	4	5	3	4	5	3	10	4	10
		3	4	8	9						
EQUIP. INDEX	-	0	28	40	43	51	63	66	74	75	87
		88	96	108	115						

EQUIPMENT NUMBER	PARAMETER NUMBER	PARAMETER VALUE
1	1	0.3000000E 01
	2	0.2700000E 02
	3	0.4100000E 02
	4	0.4200000E 02
	5	0.1106000E 04
	6	0.8000000E 01
	7	0.8000000E 01
	8	0.1500000E 01
	17	0.4000000E 02
	18	0.7200000E 02
	19	0.1046818E 00
	20	0.9000000E 01
	21	0.8957994E-01
	22	0.1400000E 02
	25	0.1850000E 04
	27	0.2500000E 03
2	1	0.1000000E 01
	2	0.2000000E 02
	3	0.1282000E 01
	4	0.1025000E 04
	5	0.6820000E 02
	7	0.7000000E 01
	10	0.1000000E 02

EQUIPMENT NUMBER	PARAMETER NUMBER	PARAMETER VALUE
5	1	0.2000000E 01
	2	0.2000000E 02
	3	0.1282000F 01
	4	0.1025000E 04
	5	0.6820000F 02
	7	0.1200000E 02
9	10	0.1000000E 02
	1	0.3000000F 01
	2	0.1600000E 02
	3	0.1282000E 01
	4	0.1025000F 04
	5	0.6820000E 02
12	7	0.1700000E 02
	10	0.1000000F 02
	1	0.4000000E 01
	2	0.2000000E 02
	3	0.1282000E 01
	4	0.1025000E 04
4	5	0.3000000E 02
	7	0.2000000E 02
	10	0.8000000F 01
	1	0.1000000E 01
7	2	0.7500000E 03
	3	0.3000000F 01
	8	0.1499999E 00
	1	0.2000000E 01
11	2	0.8000000E 03
	3	0.3000000E 01
	8	0.1499999F 00
	1	0.3000000F 01
13	2	0.7600000E 03
	3	0.3000000E 01
	8	0.1499999F 00
	1	0.3000000F 01
14	2	0.7600000E 03
	3	0.3000000E 01
	8	0.1499999F 00
	1	0.3000000F 01

END OF ALL DATA

CALCULATION SEQUENCE OPTIMIZATION

INITIAL SEQUENCE IS -

1 2 3 4 5 6 7 8 9 10 11 12 13 14

THE OPTIMIZED CALCULATION SEQUENCE IS -

1 2 3 4 5 6 7 8 9 10 11 12 13 14

NO STREAMS NEED BE ASSUMED

PRIMARY REACTION CUT-OFF TEMPERATURE (BOILER) = 1850. DEG.F

SECONDARY REACTION CUT-OFF TEMPERATURE = 1850. DEG.F

(BELOW THIS TEMPERATURE, THE LAST 4 GASEOUS
MOLECULAR SPECIES ARE MASKED FOR THE BOILER
AND THE CONVERTER COMPOSITION CALCULATIONS.)

COMBUSTION REACTION AND WASTE HEAT BOILER.
EQUIPMENT NUMBER 1

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 127.9 PRESSURE (PSIA) = 19.10
STREAM ENTHALPY (BTU.) = -0.8136710E 08

MOLE NUMBERS ARE -

CH4	-	3.95800	CO2	-	310.20776
O2	-	761.54712	N2	-	2864.86865
H2O	-	163.15106	H2S	-	1604.50000
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	0.0

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 2119.3 DEG. F
PRESSURE (PSIA.) = 19.10 (CRIT = 0.10E-03)

STREAM ENTHALPY (BTU.) = -0.8136757E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	250.38078
O2	-	0.00000	N2	-	2864.86865
H2O	-	1363.45630	H2S	-	269.49438
SO2	-	189.33513	S	-	0.02687
S2	-	571.98691	S6	-	0.00001
S8	-	0.00000	COS	-	3.44270
CS2	-	0.01302	H2	-	142.61536
CO	-	60.32903	S	-	0.0

MUFFLE FURNACE - (SIMULATION)

DIAMETER (IN.) = 72.0 RESIDENCE TIME (SEC.) = 0.492
LENGTH (FT.) = 40.0 HEAT RELEASE (BTU/CU.FT.) = 87143.

SIMULATION OF TUBE PASS NO. 1

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 1486.0 DEG. F
PRESSURE (PSIA.) = 18.92 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 8.00
NUMBER OF TUBES = 41.
TUBE LENGTH (FT.) = 27.00
PRESSURE DROP (PSI) = 0.18
TOTAL HEAT LOSS (BTU.) = 0.3792261E 08

STREAM ENTHALPY (BTU.) = -0.1193335E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13989
O2	-	0.00000	N2	-	2864.86865
H2O	-	1362.64160	H2S	-	337.79688
SO2	-	172.86217	S	-	0.00007
S2	-	545.12085	S6	-	0.01327
S8	-	0.00002	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12698
CO	-	26.52049	S	-	0.0

SIMULATION OF TUBE PASS NO. 2

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 1111.2 DEG. F
PRESSURE (PSIA.) = 18.79 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 8.00
NUMBER OF TUBES = 42.
TUBE LENGTH (FT.) = 27.00
PRESSURE DROP (PSI) = 0.13
TOTAL HEAT LOSS (BTU.) = 0.2138989E 08
STREAM ENTHALPY (BTU.) = -0.1407077E 09

MOLF NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13989
O2	-	0.00000	N2	-	2864.86865
H2O	-	1362.64160	H2S	-	337.79688
SO2	-	172.86217	S	-	0.00000
S2	-	488.04150	S6	-	18.00061
S8	-	0.77900	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12698
CO	-	26.52049	S	-	0.0

BOILER BY-PASS NO. 2 , (RATIO = 0.0896)
STREAM NUMBER 14

TEMPERATURE (DEG. F) = 1111.2 PRESSURE (PSIA) = 18.79
STREAM ENTHALPY (BTU.) = -0.1260457E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	25.45323
O2	-	0.00000	N2	-	256.63452
H2O	-	122.06534	H2S	-	30.25981
SO2	-	15.43498	S	-	0.00000
S2	-	43.71872	S6	-	1.61249
S8	-	0.06978	COS	-	0.31288
CS2	-	0.00109	H2	-	6.72987
CO	-	2.37570	S	-	0.0

BOILER BY-PASS NO. 1 , (RATIO = 0.1047)
STREAM NUMBER 9

TEMPERATURE (DEG. F) = 1111.2 PRESSURE (PSIA) = 18.79
STREAM ENTHALPY (BTU.) = -0.1341003E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	27.07977
O2	-	0.00000	N2	-	273.03467
H2O	-	129.86580	H2S	-	32.19353
SO2	-	16.47453	S	-	0.00000
S2	-	46.51253	S6	-	1.71554
S8	-	0.07424	COS	-	0.33287
CS2	-	0.00116	H2	-	7.15994
CO	-	2.52752	S	-	0.0

SIMULATION OF TUBE PASS NO. 3

ITERATIVE NON-ADIABATIC TEMPERATURE CALCULATION
TDIAM SPECIFIED, DELPC CALCULATED.

FINAL CONVERGED TEMPERATURE IS 552.0 DEG. F
PRESSURE (PSIA.) = 18.59 (CRIT = 0.10E-03)

TUBE DIA. (IN.) = 1.50
NUMBER OF TUBES = 1106.
TUBE LENGTH (FT.) = 27.00
PRESSURE DROP (PSI) = 0.21
TOTAL HEAT LOSS (BTU.) = 0.3893232E 08

BOILER EXIT STREAM -
STREAM NUMBER 6

TEMPERATURE (DEG. F) = 552.0 PRESSURE (PSIA) = 18.59
STREAM ENTHALPY (BTU.) = -0.1536236E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	231.60674
O2	-	0.00000	N2	-	2335.19897
H2O	-	1111.24487	H2S	-	274.80835
SO2	-	140.63519	S	-	0.0
S2	-	0.46069	S6	-	45.90483
S8	-	76.64828	COS	-	2.84696
CS2	-	0.00990	H2	-	61.23717
CO	-	21.61725	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 528.7
STREAM WATER DEW PT. (DEG. F) = 160.6

EQUIP. HEAT DUTY (BTU/HR) IS 0.9824482E 08

STEAM TEMP. (DEG. F.) = 401.0
PRESS. (PSIA) = 250.000
LATENT HEAT (BTU/LB) = 822.1
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.1195080E 06

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 68.00

CONDENSER 1
EQUIPMENT NUMBER 2

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 552.C PRESSURE (PSIA) = 18.59
STREAM ENTHALPY (BTU.) = -0.1536236E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	231.60674
O2	-	0.00000	N2	-	2335.19897
H2O	-	1111.24487	H2S	-	274.80835
SO2	-	140.63519	S	-	0.0
S2	-	0.46069	S6	-	45.90483
S8	-	76.64828	COS	-	2.84696
CS2	-	0.00990	H2	-	61.23717
CO	-	21.61725	S	-	0.0

CONDENSER SIMULATION

TUBE LENGTH (FT.) = 20.0
TUBE DIAMETER (IN.) = 1.282
NUMBER OF TUBES = 1025

MAXIMUM FLOW RATE (LB/SQ.FT.SFC) = 4.33
OUTLET GAS TEMPERATURE (DEG.F) = 346.3
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 14.09

EQUIP. HEAT DUTY (BTU/HR) IS 0.1162080E 08

STEAM TEMP. (DEG.F.) = 301.2
PRESS. (PSIA) = 68.200
LATENT HEAT (BTU/LB) = 908.9
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.1278543E 05

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 97.33, PERCENT RECOVERY = 38.59
SULPHUR FOG - 522.57 MOLES, OR 16722.3 LBS.
SULPHUR LIQUID - 343.25 MOLES, OR 10983.9 LBS.
(STREAM NO. 7 , TEMPERATURE = 306.3 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 10.00
EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 97.33, PERCENT RECOVERY = 95.87
SULPHUR FOG - 13.06 MOLES, OR 417.9 LBS.
SULPHUR LIQUID - 852.76 MOLES, OR 27288.2 LBS.
(STREAM NO. 7 , TEMPERATURE = 330.3 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 8

TEMPERATURE (DEG. F) = 346.3 PRESSURE (PSIA) = 18.43
STREAM ENTHALPY (BTU.) = -0.1675524E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	231.60674
O2	-	0.00000	N2	-	2335.19897
H2O	-	1111.24487	H2S	-	274.80835
SO2	-	140.63519	S	-	0.0
S2	-	0.00083	S6	-	0.64960
S8	-	2.47703	COS	-	2.84696
CS2	-	0.00990	H2	-	61.23717
CO	-	21.61725	S	-	13.06006

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 3

COMBINE STREAMS 8 AND 9

FIND GIVEN FEED STREAM RESULTANT TEMPERATURE
ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 490.0 DEG. F
PRESSURE (PSIA.) = 18.43 (CRIT = 0.10F-03)

COMBINED OUTLET STREAM (SULPHUR SHIFT DONE) -
STREAM NUMBER 10

TEMPERATURE (DEG. F) = 490.0 PRESSURE (PSIA) = 18.43
STREAM ENTHALPY (BTU.) = -0.1809630E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	258.68628
O2	-	0.00000	N2	-	2608.23364
H2O	-	1241.11060	H2S	-	307.00171
SO2	-	157.10973	S	-	0.0
S2	-	0.07465	S6	-	7.51174
S8	-	11.93349	COS	-	3.17983
CS2	-	0.01105	H2	-	68.39709
CO	-	24.14476	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 420.0
STREAM WATER DEW PT. (DEG. F) = 161.3

CONVERTER 1
EQUIPMENT NUMBER 4

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 490.0 PRESSURE (PSIA) = 18.43
STREAM ENTHALPY (BTU.) = -0.1809630E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	258.68628
O2	-	0.00000	N2	-	2608.23364
H2O	-	1241.11060	H2S	-	307.00171
SO2	-	157.10973	S	-	0.0
S2	-	0.07465	S6	-	7.51174
S8	-	11.93349	COS	-	3.17983
CS2	-	0.01105	H2	-	68.39709
CO	-	24.14476	S	-	0.0

CONVERTER BED (SIMULATION)

CROSSECTIONAL AREA (SQ.FT) = 750.00
THICKNESS (FT.) = 3.00
VOLUME (CU.FT.) = 2250.00
LINEAR GAS VELOCITY (FT./SEC.) = 1.00
MOLAL FLOW RATE (MOLE/HR.SQ.FT.) = 2.08
AVERAGE PARTICLE DIAMETER (IN.) = 0.15
PRESSURE DROP (PSI.) = 0.402

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 607.9 DEG. F
PRESSURE (PSIA.) = 18.03 (CRIT = 0.10E-03)

CONVERTER DEW POINT CHECK -

BED TEMPERATURE	DEW POINT TEMPERATURE	TEMPERATURE DIFFERENCE	BED PRESSURE
513.548	438.620	74.928	18.351
537.129	453.013	84.117	18.271
560.710	464.945	95.765	18.190
584.292	475.252	109.039	18.110
607.873	484.459	123.413	18.029

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 75.68

PERCENT OF NON-ELEMENTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 68.36

CONVERTER EXIT STREAM -
STREAM NUMBER 11

TEMPERATURE (DEG. F) = 607.9 PRESSURE (PSIA) = 18.03
STREAM ENTHALPY (BTU.) = -0.1809604E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	258.68628
O2	-	0.0	N2	-	2608.23364
H2O	-	1454.07959	H2S	-	94.03189
SO2	-	50.62482	S	-	0.0
S2	-	1.28281	S6	-	34.52592
S8	-	31.30252	COS	-	3.17983
CS2	-	0.01105	H2	-	68.39709
CO	-	24.14476	S	-	0.0

CONDENSER 2
EQUIPMENT NUMBER 5

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 607.9 PRESSURE (PSIA) = 18.03
STREAM ENTHALPY (BTU.) = -0.1809604E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	258.68628
O2	-	0.0	N2	-	2608.23364
H2O	-	1454.07959	H2S	-	94.03189
SO2	-	50.62482	S	-	0.0
S2	-	1.28281	S6	-	34.52592
S8	-	31.30252	COS	-	3.17983
CS2	-	0.01105	H2	-	68.39709
CO	-	24.14476	S	-	0.0

CONDENSER SIMULATION

TUBE LENGTH (FT.) = 20.0
TUBE DIAMETER (IN.) = 1.282
NUMBER OF TUBES = 1025

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.01
OUTLET GAS TEMPERATURE (DEG.F) = 342.2
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 13.46

EQUIP. HEAT DUTY (BTU/HR) IS 0.1223156E 08

STEAM TEMP. (DEG.F.) = 301.2
PRESS. (PSIA) = 68.200
LATENT HEAT (BTU/LB) = 908.9
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.1345740E 05

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 94.70, PERCENT RECOVERY = 50.69
SULPHUR FOG - 202.51 MOLES, OR 6480.3 LBS.
SULPHUR LIQUID - 233.24 MOLES, OR 7463.7 LBS.
(STREAM NO. 12 , TEMPERATURE = 307.1 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 10.00

EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 94.70, PERCENT RECOVERY = 91.60
SULPHUR FOG - 14.25 MOLES, OR 456.1 LBS.
SULPHUR LIQUID - 421.50 MOLES, OR 13487.9 LBS.
(STREAM NO. 12 , TEMPERATURE = 322.9 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 13

TEMPERATURE (DEG. F) = 342.2 PRESSURE (PSIA) = 17.85
STREAM ENTHALPY (BTU.) = -0.1943174E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	258.68628
O2	-	0.0	N2	-	2608.23364
H2O	-	1454.07959	H2S	-	94.03189
SO2	-	50.62482	S	-	0.0
S2	-	0.00087	S6	-	0.67331
S8	-	2.54327	COS	-	3.17983
CS2	-	0.01105	H2	-	68.39709
CO	-	24.14476	S	-	14.25429

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 6

COMBINE STREAMS 13 AND 14

FIND GIVEN FEED STREAM RESULTANT TEMPERATURE
ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 470.0 DEG. F
PRESSURE (PSIA.) = 17.85 (CRIT = 0.10E-03)

COMBINED OUTLET STREAM (SULPHUR SHIFT DONE) -
STREAM NUMBER 15

TEMPERATURE (DEG. F) = 470.0 PRESSURE (PSIA) = 17.85
STREAM ENTHALPY (BTU.) = -0.2069217E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1576.14478	H2S	-	124.29170
SO2	-	66.10979	S	-	0.0
S2	-	0.04886	S6	-	6.64599
S8	-	12.04237	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

STREAM SULPHUR DEW PT. (DEG. F) = 413.2
STREAM WATER DEW PT. (DEG. F) = 167.0

CONVERTER 2
EQUIPMENT NUMBER 7

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 470.0 PRESSURE (PSIA) = 17.85
STREAM ENTHALPY (BTU.) = -0.2069217E 09

MOLF NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1576.14478	H2S	-	124.29170
SO2	-	66.10979	S	-	0.0
S2	-	0.04886	S6	-	6.64599
S8	-	12.04237	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

CONVERTER BED (SIMULATION)

CROSSECTIONAL AREA (SQ.FT) = 800.00
THICKNESS (FT.) = 3.00
VOLUME (CU.FT.) = 2400.00
LINEAR GAS VELOCITY (FT./SEC.) = 1.02
MOLAL FLOW RATE (MOLE/HR.SQ.FT.) = 2.10
AVERAGE PARTICLE DIAMETER (IN.) = 0.15
PRESSURE DROP (PSI.) = 0.366

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 511.4 DEG. F
PRESSURE (PSIA.) = 17.49 (CRIT = 0.10E-03)

CONVERTER DEW POINT CHECK -

BED TEMPERATURE	DEW POINT TEMPERATURE	TEMPERATURE DIFFERENCE	BED PRESSURE
478.263	420.483	57.781	17.781
486.552	426.946	59.607	17.708
494.842	432.762	62.080	17.635
503.131	438.059	65.072	17.562
511.420	442.930	68.489	17.488

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 76.18

PERCENT OF NON-ELEMENTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 59.43

CONVERTER EXIT STREAM -
STREAM NUMBER 16

TEMPERATURE (DEG. F) = 511.4 PRESSURE (PSIA) = 17.49
STREAM ENTHALPY (BTU.) = -0.2069212E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1652.97705	H2S	-	47.45825
SO2	-	27.69304	S	-	0.0
S2	-	0.15809	S6	-	13.87646
S8	-	20.99840	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

BLACK BOX
EQUIPMENT NUMBER 8

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 511.4 PRESSURE (PSIA) = 17.49
STREAM ENTHALPY (BTU.) = -0.2069212E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1652.97705	H2S	-	47.45825
SO2	-	27.69304	S	-	0.0
S2	-	0.15809	S6	-	13.87646
S8	-	20.99840	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

TEMPERATURE CHANGED FROM 511.4 TO 383.0 DEG.F.

(ENTHALPY DIFFERENCE IS -0.520341E 07 BTU/HR.)

STREAM NUMBER 30

TEMPERATURE (DEG. F) = 383.0 PRESSURE (PSIA) = 17.70
STREAM ENTHALPY (BTU.) = -0.2121246E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1652.97705	H2S	-	47.45825
SO2	-	27.69304	S	-	0.0
S2	-	0.00510	S6	-	5.72653
S8	-	27.14906	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

CONDENSER 3
EQUIPMENT NUMBER 9

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 383.0 PRESSURE (PSIA) = 17.70
STREAM ENTHALPY (BTU.) = -0.2121246E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1652.97705	H2S	-	47.45825
SO2	-	27.69304	S	-	0.0
S2	-	0.00510	S6	-	5.72653
S8	-	27.14906	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

CONDENSER SIMULATION

TUBE LENGTH (FT.) = 16.0
TUBE DIAMETER (IN.) = 1.282
NUMBER OF TUBES = 1025

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.08
OUTLET GAS TEMPERATURE (DEG.F) = 320.7
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 14.62

EQUIP. HEAT DUTY (BTU/HR) IS 0.3491473E 07

STEAM TEMP. (DEG.F.) = 301.2
PRESS. (PSIA) = 68.200
LATENT HEAT (BTU/LB) = 908.9
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.3841387E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 94.04, PERCENT RECOVERY = 32.58

SULPHUR FOG - 154.60 MOLES, OR 4947.4 LBS.

SULPHUR LIQUID - 81.95 MOLES, OR 2622.5 LBS.

(STREAM NO. 17, TEMPERATURE = 303.6 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 10.00EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 94.04, PERCENT RECOVERY = 87.85

SULPHUR FOG - 15.57 MOLES, OR 498.2 LBS.

SULPHUR LIQUID - 220.99 MOLES, OR 7071.6 LBS.

(STREAM NO. 17, TEMPERATURE = 314.4 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 31

TEMPERATURE (DEG. F) = 320.7 PRESSURE (PSIA) = 17.56

STREAM ENTHALPY (BTU.) = -0.2161872E 09

MOLE NUMBERS ARE -

CH4 -	0.00000	CO2 -	284.13940
O2 -	0.00000	N2 -	2864.86816
H2O -	1652.97705	H2S -	47.45825
SO2 -	27.69304	S -	0.0
S2 -	0.00039	S6 -	0.38483
S8 -	1.58685	COS -	3.49270
CS2 -	0.01214	H2 -	75.12695
CO -	26.52046	S -	15.56963

BLACK BOX
EQUIPMENT NUMBER 10

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 320.7 PRESSURE (PSIA) = 17.56
STREAM ENTHALPY (BTU.) = -0.2161872E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1652.97705	H2S	-	47.45825
SO2	-	27.69304	S	-	0.0
S2	-	0.00039	S6	-	0.38483
S8	-	1.58685	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	15.56963

TEMPERATURE CHANGED FROM 320.7 TO 388.0 DEG.F.
(ENTHALPY DIFFERENCE IS 0.265944E 07 BTU/HR.)

STREAM NUMBER 18

TEMPERATURE (DEG. F) = 388.0 PRESSURE (PSIA) = 17.20
STREAM ENTHALPY (BTU.) = -0.2135277E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1652.97705	H2S	-	47.45825
SO2	-	27.69304	S	-	0.0
S2	-	0.00348	S6	-	1.14639
S8	-	2.96111	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

CONVERTER 3
EQUIPMENT NUMBER 11

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 388.0 PRESSURE (PSIA) = 17.20
STREAM ENTHALPY (BTU.) = -0.2135277F 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1652.97705	H2S	-	47.45825
SO2	-	27.69304	S	-	0.0
S2	-	0.00348	S6	-	1.14639
S8	-	2.96111	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

CONVERTER BED (SIMULATION)

CROSSECTIONAL AREA (SQ.FT) = 760.00
THICKNESS (FT.) = 3.00
VOLUME (CU.FT.) = 2280.00
LINEAR GAS VELOCITY (FT./SEC.) = 1.00
MOLAL FLOW RATE (MOLE/HR.SQ.FT.) = 2.19
AVERAGE PARTICLE DIAMETER (IN.) = 0.15
PRESSURE DROP (PSI.) = 0.364

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 406.6 DEG. F
PRESSURE (PSIA.) = 16.84 (CRIT = 0.10E-03)

CONVERTER DEW POINT CHECK -

BED TEMPERATURE	DEW POINT TEMPERATURE	TEMPERATURE DIFFERENCE	BED PRESSURE
391.711	358.839	32.872	17.127
395.422	367.167	28.254	17.054
TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
399.132	374.226	24.906	16.982
TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
402.843	380.334	22.509	16.909
TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
406.554	385.727	20.827	16.836

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 72.50

PERCENT OF NON-ELEMENTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 61.81

CONVERTER EXIT STREAM -
STREAM NUMBER 19

TEMPERATURE (DEG. F) = 406.6 PRESSURE (PSIA) = 16.84
STRFAM ENTHALPY (BTU.) = -0.2135274E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1685.39478	H2S	-	15.03993
SO2	-	11.48389	S	-	0.0
S2	-	0.00788	S6	-	2.82569
S8	-	7.77897	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

CONDENSER 4
EQUIPMENT NUMBER 12

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 406.6 PRESSURE (PSIA) = 16.84
STREAM ENTHALPY (BTU.) = -0.2135274E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1685.39478	H2S	-	15.03993
SO2	-	11.48389	S	-	0.0
S2	-	0.00788	S6	-	2.82569
S8	-	7.77897	CDS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	0.0

CONDENSER SIMULATION

TUBE LENGTH (FT.) = 20.0
TUBE DIAMETER (IN.) = 1.282
NUMBER OF TUBES = 1025

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 3.87
OUTLET GAS TEMPERATURE (DEG.F) = 268.5
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 12.82

EQUIP. HEAT DUTY (BTU/HR) IS 0.5656767E 07

STEAM TEMP. (DEG.F.) = 250.4
PRESS. (PSIA) = 30.000
LATENT HEAT (BTU/LB) = 947.9
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.5967910E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 96.01, PERCENT RECOVERY = 32.21

SULPHUR FOG - 50.53 MOLES, OR 1616.9 LBS.
SULPHUR LIQUID - 25.51 MOLES, OR 816.5 LBS.
(STREAM NO. 20 , TEMPERATURE = 252.4 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 8.00

EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 96.01, PERCENT RECOVERY = 80.34

SULPHUR FOG - 12.42 MOLES, OR 397.3 LBS.
SULPHUR LIQUID - 63.63 MOLES, OR 2036.1 LBS.
(STREAM NO. 20 , TEMPERATURE = 262.1 DEG.F.)

CONDENSER GASFOUS EXIT STREAM
STREAM NUMBER 21

TEMPERATURE (DEG. F) = 268.5 PRESSURE (PSIA) = 16.66
STREAM ENTHALPY (BTU.) = -0.2193183F 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1685.39478	H2S	-	15.03993
SO2	-	11.43389	S	-	0.0
S2	-	0.00004	S6	-	0.06724
S8	-	0.34438	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	12.41518

EXHAUST GAS INCINERATOR
EQUIPMENT NUMBER 13

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 268.5 PRESSURE (PSIA) = 16.66
STREAM ENTHALPY (BTU.) = -0.2193183E 09

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	284.13940
O2	-	0.00000	N2	-	2864.86816
H2O	-	1685.39478	H2S	-	15.03993
SO2	-	11.48389	S	-	0.0
S2	-	0.00004	S6	-	0.06724
S8	-	0.34438	COS	-	3.49270
CS2	-	0.01214	H2	-	75.12695
CO	-	26.52046	S	-	12.41518

FUEL AND AIR STREAM
STREAM NUMBER 27

TEMPERATURE (DEG. F) = 72.0 PRESSURE (PSIA) = 15.00
STREAM ENTHALPY (BTU.) = -0.5601844E 07

MOLE NUMBERS ARE -

CH4	-	107.61998	CO2	-	0.0
O2	-	386.63965	N2	-	1454.48975
H2O	-	19.86998	H2S	-	0.0
SO2	-	0.0	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.0
CO	-	0.0	S	-	0.0

ITERATIVE ADIABATIC TEMPERATURE CALCULATION

FINAL CONVERGED TEMPERATURE IS 1200.4 DEG. F
PRESSURE (PSIA.) = 16.66 (CRIT = 0.10E-03)

INCINERATOR EXHAUST STREAM
STREAM NUMBER 23

TEMPERATURE (DEG. F) = 1200.4 PRESSURE (PSIA) = 16.66
STEAM ENTHALPY (BTU.) = -0.2249201E 09

MOLE NUMBERS ARE -

CH4	-	0.0	CO2	-	421.78345
O2	-	77.16615	N2	-	4319.35547
H2O	-	2010.67139	H2S	-	0.0
SO2	-	45.61459	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.00000
CO	-	0.00000	S	-	0.0

SULPHUR PLANT STACK
EQUIPMENT NUMBER 14

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 1200.4 PRESSURE (PSIA) = 16.66
STREAM ENTHALPY (BTU.) = -0.2249201E 09

MOLE NUMBERS ARE -

CH4	-	0.0	CO2	-	421.78345
O2	-	77.16615	N2	-	4319.35547
H2O	-	2010.67139	H2S	-	0.0
SO2	-	45.61459	S	-	0.0
S2	-	0.0	S6	-	0.0
S8	-	0.0	COS	-	0.0
CS2	-	0.0	H2	-	0.00000
CO	-	0.00000	S	-	0.0

SULPHUR PLANT STACK SIMULATION

AMBIENT TEMPERATURE (DEG.F) = 80.0
EQUIVALENT STACK TEMPERATURE (DEG.F) = 72.7
TOTAL GASEOUS STACK FLOWRATE (C.F.S. AT TEQIV) = 655.0
POLLUTANT (SO2) FLOWRATE (C.F.S. AT TEQIV) = 4.346
STACK OUTLET TEMPERATURE (DEG.F) = 1000.4

STACK DIAMETER (FT. AT TOP) = 3.70
STACK VELOCITY (FT/SEC. AT TOP) = 60.92

ATMOSPHERIC CONDITIONS

STABLE UNSTABLE

STACK HEIGHT (FT.) =	130.0	130.0
MAX. GROUND CONCENTRATION (PPM) =	0.2011	0.1661
WIND SPEED AT MAX. (FT/SEC) =	14.67	20.00
DISTANCE (SOURCE TO MAX., FT.) =	8312.	3136.
EFFECTIVE STACK HEIGHT (FT.) =	415.6	313.6

EXAMPLE 4.

SPECIFICATIONS

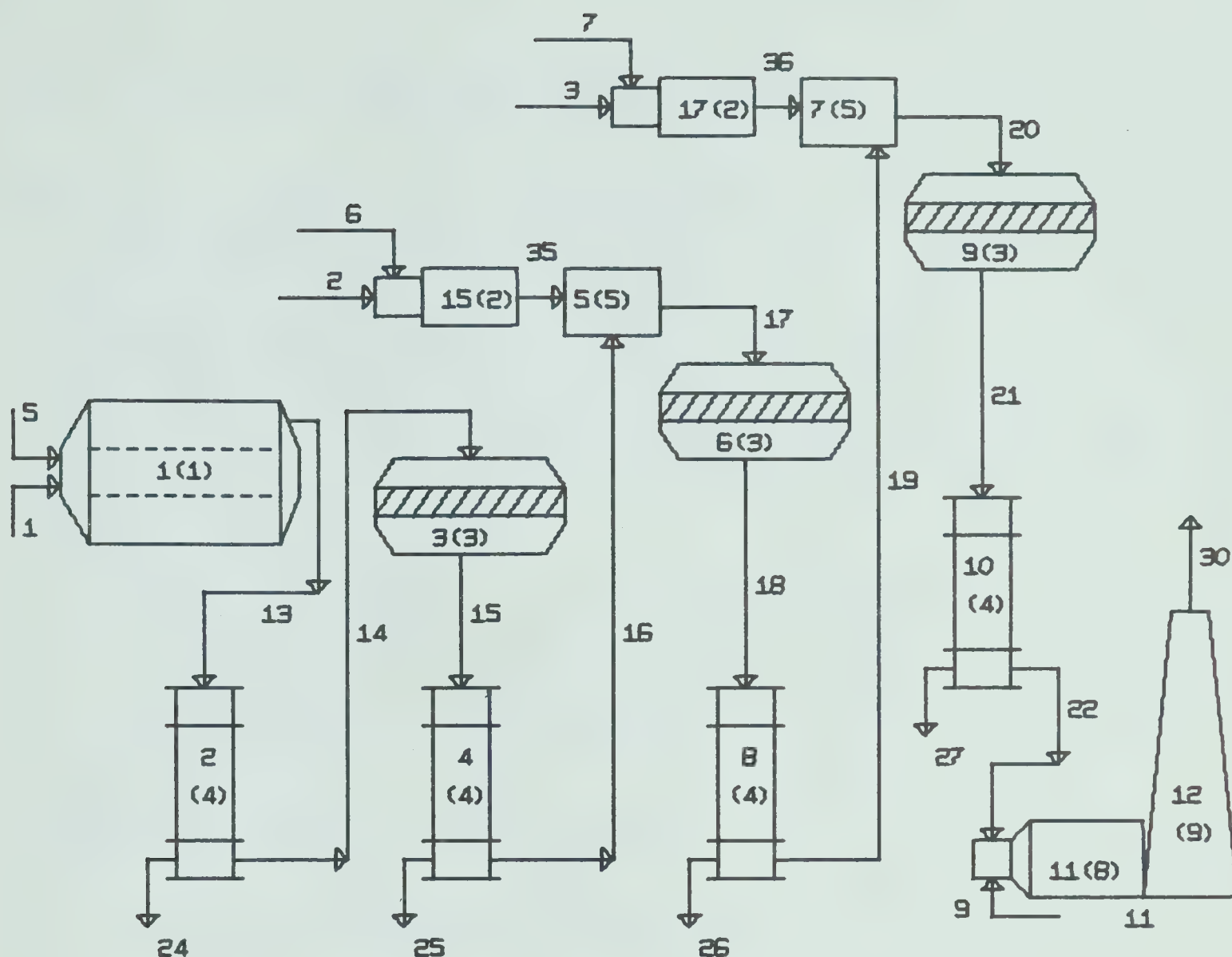
PLANT FEEDS

	BOILER FEED	NO. 1 INLINE BURNER	NO. 2 INLINE BURNER	INCINERATOR
CH ₄	33.5	14.167	19.375	278.3
CO ₂	1330.88	23.17	19.04	
CO _S	1.13			
H ₂ O	132.4	2.29	1.875	
H ₂ S	3100.1	54.	44.33	
O ₂	1396.7	44.75	35.83	880.5
N ₂	5270.	168.96	135.5	3321.7

SPECIFIED TEMPERATURES AND PRESSURES	DEG.F.	PSIA.
AMBIENT	45.	
BOILER ACID GAS FEED	82.	19.
BOILER COMBUSTION AIR	139.	20.3
INLINE BURNERS' FUEL AND ACID GAS FEEDS	120.	19.
INLINE BURNERS' COMBUSTION AIR	139.	20.
INCINERATOR AIR AND FUEL GAS	100.	20.
BOILER EXIT	700.	
PRIMARY (BOILER) EQUILIBRIUM CUTOFF	2000.	
SECONDARY (MASKING) EQUILIBRIUM CUTOFF	2000.	
NO. 1 CONDENSER EXIT	445.	
NO. 2 CONDENSER EXIT	350.	
NO. 3 CONDENSER EXIT	339.	
NO. 4 CONDENSER EXIT	282.	

MISCELLANEOUS

- 2 PASS BOILER 30 FT. LONG
- MINIMUM FLAME REACTION RESIDENCE TIME 0.6 SEC. (BOILER) AND 0.5 SEC. (INLINE BURNERS)
- MAX. FOG IN 1ST, 2ND, 3RD, AND 4TH CONDENSERS 10, 5, 3, AND 3 LB. SULPHUR/100 MOLES INERT EXIT GAS RESPECTIVELY



LEGEND

NUMBERS DENOTE STREAM OR EQUIPMENT NUMBERS

NUMBERS IN BRACKETS DENOTE EQUIPMENT TYPES -

- | | |
|------------------------|---------------------|
| 1. WASTE HEAT BOILER | 6. COMBINER/DIVIDER |
| 2. INLINE BURNER | 7. AIR ADDER |
| 3. CATALYTIC CONVERTER | 8. INCINERATOR |
| 4. SULPHUR CONDENSER | 9. EFFLUENT STACK |
| 5. ADIABATIC COMBINER | 10. BLACK BOX |

FIG. E-4

EQUIPMENT MODULE (PROCESS)
FLOWSHEET FOR EXAMPLE 4.

PROGRAM DATA (CARD IMAGE)

```

C          EXAMPLE 4.    (SIMULATION)
*PROGRAM CONTROL PARAMETERS*
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
*END*
*FLOWSHEET DATA*
1 0 1**5 0 1**9 0 11**2 0 15**6 0 15**3 0 17**7 0 17**
35 15 5**36 17 7**
11 11 12**13 1 2**14 2 3**15 3 4**16 4 5**17 5 6**18 6 8**
19 8 7**20 7 9**21 9 10**22 10 11**24 2 0**25 4 0**26 8 0**
27 10 0**30 12 0**
*END*
*STREAM SPECIFICATIONS*
1 1 33.5 2 1330.88 12 1.125 6 3100.1 5 132.4 21 82. 22 19.**
5 3 1396.7 4 5270. 21 139. 22 20.3**
2 4 .25 1 14.167 2 23.17 6 54. 5 2.29 21 120. 22 19. **
6 3 44.75 4 168.71 21 139. 22 20.**
3 4 .333 1 19.375 2 19.04 6 44.33 5 1.875 21 120. 22 19. **
7 3 35.83 4 135.17 21 139. 22 20.**
9 1 278.3 3 880.5 4 3321.7 21 100. 22 20.**
*END*
*EQUIPMENT PARAMETER SPECIFICATIONS*
1 1, 2 4, 3 3, 4 4, 5 5, 6 3, 7 5, 8 4, 9 3, 10 4, 11 8, 12 9
15 2, 17 2 **
1 1 2. 2 30. 10 700. 15 .6 25 2000. **
2 1 1. 7 24. 8 445. 10 10.**
3 1 1.**
4 1 2. 7 25. 8 350. 10 5.**
6 1 2.**
8 1 3. 7 26. 8 339. 10 3.**
9 1 3.**
10 1 4. 7 27. 8 282. 10 3.**
11 7 9.**
12 1 45.**
15 3 .5**
17 3 .5**
*END*
C          MOLECULAR AND THERMODYNAMIC DATA SAME AS EXAMPLE 1.

```


SULPHUR PLANT DESIGN AND SIMULATION

PROGRAM CONTROL PARAMETERS

END

FLOWSHEET DATA

END

STREAM SPECIFICATIONS

END

EQUIPMENT PARAMETER SPECIFICATIONS

END

MOLECULAR AND THERMODYNAMIC DATA

END OF ALL DATA

CALCULATION SEQUENCE OPTIMIZATION

INITIAL SEQUENCE IS -

1 2 3 4 5 6 7 8 9 10 11 12 15 17

THE OPTIMIZED CALCULATION SEQUENCE IS -

1 2 3 4 15 17 5 6 8 7 9 10 11 12

NO STREAMS NEED BE ASSUMED

PRIMARY REACTION CUT-OFF TEMPERATURE (BOILER) = 2000. DEG.F

SECONDARY REACTION CUT-OFF TEMPERATURE = 2000. DEG.F

(BELOW THIS TEMPERATURE, THE LAST 4 GASFOUS
MOLECULAR SPECIES ARE MASKED FOR THE BOILER
AND THE CONVERTER COMPOSITION CALCULATIONS.)

COMBUSTION REACTION AND WASTE HEAT BOILER.

EQUIPMENT NUMBER 1

CONDENSER 1
EQUIPMENT NUMBER 2

CONVERTER 1
EQUIPMENT NUMBER 3

TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
467.429	459.590	7.839	18.432
TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
489.853	469.841	20.017	18.403

CONDENSER 2
EQUIPMENT NUMBER 4

INLINE BURNER.
EQUIPMENT NUMBER 15

INLINE BURNER.
EQUIPMENT NUMBER 17

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 5

CONVERTER 2
EQUIPMENT NUMBER 6

CONDENSER 3
EQUIPMENT NUMBER 8

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 7

CONVERTER 3
EQUIPMENT NUMBER 9

CONDENSER 4
EQUIPMENT NUMBER 10

EXHAUST GAS INCINERATOR
EQUIPMENT NUMBER 11

SULPHUR PLANT STACK
EQUIPMENT NUMBER 12

OVERALL PLANT MASS AND ENERGY BALANCE

ATOM AND TOTAL MASS BALANCES

ATOM TYPE	ATOM TOTAL	PERCENT ERROR
S	0.319955E 04	0.00075
O	0.759942E 04	0.0
C	0.171956E 04	0.00003
H	0.805136E 04	0.00015
N	0.177923E 05	0.0
TOTAL	0.383622E 05	0.00009

ENERGY BALANCE

(ENTHALPY IS RELATIVE AND IN BTU.)

ENTHALPY IN = -0.281556E 09

ENTHALPY OUT = -0.556069E 09

DIFFERENCE = 0.274513E 09

DIFFERENCE SHOULD BE TOTAL PLANT HEAT LOAD

OVERALL PLANT SULPHUR RECOVERY

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 97.23

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 1				WASTE HEAT BOILER			
1 =	0.200000E	01	*	2 =	0.300000E	02	*
3 =	0.361000E	03		4 =	0.445000E	03	
5 =	0.0			6 =	0.400000E	01	*
7 =	0.300000E	01	*	8 =	0.0		
9 =	0.989243E	03		10 =	0.699968E	03	*
11 =	0.0			12 =	0.179077E	00	
13 =	0.280899E	00		14 =	0.0		
15 =	0.268891E	00	*	16 =	0.157345E	06	
17 =	0.400000E	02		18 =	0.720000E	02	
19 =	0.0			20 =	0.0		
21 =	0.0			22 =	0.0		
23 =	0.0			24 =	0.0		
25 =	0.200000E	04	*	26 =	0.190698E	04	
27 =	0.250000E	03		28 =	0.170248E	09	

EQUIPMENT NUMBER 2				CONDENSER			
1 =	0.100000E	01	*	2 =	0.751564E	01	
3 =	0.100000E	01		4 =	0.457400E	04	
5 =	0.500000E	02		6 =	0.399958E	01	
7 =	0.240000E	02	*	8 =	0.445000E	03	*
9 =	0.0			10 =	0.100000E	02	*
11 =	0.745890E	02		12 =	0.336151E	08	

EQUIPMENT NUMBER 3				CONVERTER			
1 =	0.100000E	01	*	2 =	0.156811E	04	
3 =	0.300000E	01		4 =	0.470432E	04	
5 =	0.147468E	00		6 =	0.100000E	01	
7 =	0.219677E	01		8 =	0.500000E	00	

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 4

CONDENSER

1 = 0.200000E 01 *	2 = 0.107707E 02
3 = 0.100000E 01	4 = 0.390700E 04
5 = 0.500000E 02	6 = 0.399961E 01
7 = 0.250000E 02 *	8 = 0.350000E 03 *
9 = 0.0	10 = 0.500000E 01 *
11 = 0.937232E 02	12 = 0.233539E 08

EQUIPMENT NUMBER 15

IN-LINE BURNER

1 = 0.160000E 02	2 = 0.360000E 02
3 = 0.810600E 00 *	4 = 0.539612E 05
5 = 0.235111E 04	

EQUIPMENT NUMBER 17

IN-LINE BURNER

1 = 0.160000E 02	2 = 0.360000E 02
3 = 0.100448E 01 *	4 = 0.422915E 05
5 = 0.217703E 04	

EQUIPMENT NUMBER 5

ADIABATIC COMBINER

1 = 0.0	2 = 0.427293E 03
3 = 0.0	

EQUIPMENT NUMBER 6

CONVERTER

1 = 0.200000E 01 *	2 = 0.155891E 04
3 = 0.300000E 01	4 = 0.467673E 04
5 = 0.123546E 00	6 = 0.100000E 01
7 = 0.220678E 01	8 = 0.500000E 00

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 8

CONDENSER

1 = 0.300000E 01 *	2 = 0.745528E 01
3 = 0.100000E 01	4 = 0.355500E 04
5 = 0.500000E 02	6 = 0.399975E 01
7 = 0.260000E 02 *	8 = 0.339000E 03 *
9 = 0.0	10 = 0.300000E 01 *
11 = 0.784433E 02	12 = 0.104807E 08

EQUIPMENT NUMBER 7

ADIABATIC COMBINER

1 = 0.0	2 = 0.397639E 03
3 = 0.0	

EQUIPMENT NUMBER 9

CONVERTER

1 = 0.300000E 01 *	2 = 0.155674E 04
3 = 0.300000E 01	4 = 0.467022E 04
5 = 0.124727E 00	6 = 0.100000E 01
7 = 0.225368E 01	8 = 0.500000E 00

EQUIPMENT NUMBER 10

CONDENSER

1 = 0.400000E 01 *	2 = 0.162759E 02
3 = 0.100000E 01	4 = 0.356700E 04
5 = 0.500000E 02	6 = 0.399972E 01
7 = 0.270000E 02 *	8 = 0.291055E 03 *
9 = 0.0	10 = 0.300000E 01 *
11 = 0.834170E 02	12 = 0.101124E 08

EQUIPMENT NUMBER 11

INCINERATOR

1 = 0.0	2 = 0.0
3 = 0.0	4 = 0.0
5 = 0.0	6 = 0.0
7 = 0.900000E 01 *	

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 12

STACK

1 =	0.450000E 02 *	2 =	0.133725E 04
3 =	0.113436E 03	4 =	0.514667E 01
5 =	0.200000E 00	6 =	0.600000E 02
7 =	0.200000E 02	8 =	0.100000E 01

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE - COMPOSITION - MOLES/HR.
ENTHALPY - MMBTU./HR. VOLUME - CU.FT./MIN. (GAS ONLY)
TEMPERATURE - DEG.F. PRESSURE - PSIA.

STREAM NO.	1	2	3	5	6
CH4	33.5000	14.1670	19.3750	0.0	0.0
CO2	1330.8796	23.1700	19.0400	0.0	0.0
O2	0.0	0.0	0.0	1396.7000	44.7500
N2	0.0	0.2500	0.3330	5270.0000	168.7100
H2O	132.4000	2.2900	1.8750	0.0	0.0
H2S	3100.0999	54.0000	44.3300	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0
S2	0.0	0.0	0.0	0.0	0.0
S6	0.0	0.0	0.0	0.0	0.0
S8	0.0	0.0	0.0	0.0	0.0
COS	1.1250	0.0	0.0	0.0	0.0
CS2	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0
TOT. MOLES	4598.000	93.877	84.953	6666.699	213.460
TOT. LBS.	166948.7	3130.4	2698.1	192254.4	6155.9
TOT.LB.S(M)	0.0	0.0	0.0	0.0	0.0
TOT.LB.S(E)	99239.2	1728.0	1418.6	0.0	0.0
ENTHALPY	-266.930	-5.051	-4.396	2.886	0.092
VOLUME	23443.1	512.2	463.5	35161.3	1142.7
TEMPERATURE	82.00	120.00	120.00	139.00	139.00
S. DEW PT.	0.0	0.0	0.0	0.0	0.0
PRESSURE	19.00	19.00	19.00	20.30	20.00

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE - COMPOSITION - MOLES/HR.
ENTHALPY - MMRTU./HR. VOLUME - CU.FT./MIN. (GAS ONLY)
TEMPERATURE - DEG.F. PRESSURE - PSIA.

STREAM NO.	7	9	11	13	14
CH4	0.0	278.2998	0.0000	0.0000	0.0000
CO2	0.0	0.0	1710.1897	1143.6404	1143.6404
O2	35.8300	880.5000	0.0000	0.0000	0.0000
N2	135.1700	3321.7000	8896.1563	5270.0000	5270.0000
H2O	0.0	0.0	4000.7864	2485.9543	2485.9543
H2S	0.0	0.0	4.0386	593.3943	593.3943
SO2	0.0	0.0	84.4457	296.8247	296.8247
S	0.0	0.0	0.0000	0.0	0.0
S2	0.0	0.0	0.2023	16.8574	0.0602
S6	0.0	0.0	0.0	195.2364	19.0666
S8	0.0	0.0	0.0	123.6637	51.3909
COS	0.0	0.0	0.0516	16.4231	16.4231
CS2	0.0	0.0	0.0000	0.0656	0.0656
H2	0.0	0.0	20.8501	220.1507	220.1507
CO	0.0	0.0	9.3141	205.3755	205.3755
S	0.0	0.0	0.0	0.0	31.9746
TOT. MOLES	171.000	4480.496	14726.020	10567.563	10334.301
TOT. LBS.	4931.3	125636.3	402215.1	359202.5	306824.3
TOT.LB.S(M)	0.0	0.0	12.0	70222.1	17843.9
TOT.LB.S(E)	0.0	0.0	2846.1	99238.9	46860.6
ENTHALPY	0.074	-8.231	-537.573	-434.131	-472.505
VOLUME	915.4	22422.9	297698.4	118169.6	90284.3
TEMPERATURE	139.00	100.00	1537.25	699.97	445.00
S. DEW PT.	0.0	0.0	251.33	535.64	444.69
PRESSURE	20.00	20.00	17.67	18.55	18.46

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE - COMPOSITION - MOLES/HR.
ENTHALPY - MMBTU./HR. VOLUME - CU.FT./MIN. (GAS ONLY)
TEMPERATURE - DEG.F. PRESSURE - PSIA.

STREAM NO.	15	16	17	18	19
CH4	0.0	0.0	0.0000	0.0000	0.0000
CO2	1143.6404	1143.6404	1167.7915	1167.7915	1167.7915
O2	0.0000	0.0000	0.0000	0.0000	0.0000
N2	5270.0000	5270.0000	5438.9570	5438.9570	5438.9570
H2O	2934.8718	2934.8718	2998.3010	3099.2256	3099.2256
H2S	144.4763	144.4763	153.7638	52.8388	52.8388
SO2	72.3655	72.3655	78.9723	28.5097	28.5097
S	0.0	0.0	0.0	0.0	0.0
S2	1.0782	0.0020	0.0253	0.0653	0.0013
S6	72.2747	1.6542	5.0452	11.8472	1.2359
S8	99.3992	6.4623	10.5918	24.4037	5.0505
COS	16.4231	16.4231	16.7342	16.7342	16.7342
CS2	0.0656	0.0656	0.0667	0.0667	0.0667
H2	220.1507	220.1507	232.0580	232.0580	232.0580
CO	205.3755	205.3755	218.2491	218.2491	218.2491
S	0.0	15.6365	0.0	0.0	9.6135
TOT. MOLES	10180.102	10031.098	10320.531	10290.719	10270.305
TOT. LBS.	306824.3	269904.8	279190.8	279190.8	272502.5
TOT.LB.S(M)	39391.9	2472.4	3681.8	8526.2	1837.9
TOT.LB.S(E)	46860.6	9941.1	11669.1	11669.1	4980.8
ENTHALPY	-472.383	-498.712	-503.670	-503.669	-514.667
VOLUME	101079.6	79702.8	89970.7	93062.8	81508.6
TEMPERATURE	557.15	350.00	427.29	454.18	339.00
S. DEW PT.	494.69	349.91	374.70	411.31	339.18
PRESSURE	18.31	18.20	18.20	18.07	17.98

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE -

ENTHALPY - MMBTU./HR.

TEMPERATURE - DEG.F.

COMPOSITION - MOLES/HR.

VOLUME - CU.FT./MIN. (GAS ONLY)

PRESSURE - PSIA.

STREAM NO.	20	21	22	24	25
CH4	0.0000	0.0000	0.0000	0.0	0.0
CO2	1188.8562	1188.8562	1188.8562	0.0	0.0
O2	0.0000	0.0	0.0	0.0	0.0
N2	5574.4570	5574.4570	5574.4570	0.0	0.0
H2O	3149.7458	3183.4958	3183.4958	0.0	0.0
H2S	70.7452	36.9944	36.9944	0.0	0.0
SO2	29.3190	12.4436	12.4436	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0
S2	0.0101	0.0151	0.0002	0.0	0.0
S6	3.1403	4.9233	0.2661	0.0	0.0
S8	7.9533	12.9431	1.3295	0.0	0.0
COS	17.2871	17.2871	17.2871	0.0	0.0
CS2	0.0707	0.0707	0.0707	0.0	0.0
H2	248.5859	248.5859	248.5859	0.0	0.0
CO	235.0422	235.0422	235.0422	0.0	0.0
S	0.0	0.0	9.8411	1636.8123	1153.7310
TOT. MOLES	10525.188	10515.090	10508.648	1636.812	1153.731
TOT. LBS.	280131.7	280131.7	276578.4	52378.0	36919.4
TOT.LB.S(M)	2639.6	4259.7	706.4	52378.0	36919.4
TOT.LB.S(E)	6399.4	6399.4	2846.1	52378.0	36919.4
ENTHALPY	-518.989	-518.985	-529.341	4.643	2.917
VOLUME	89748.3	91238.6	79791.6	*****	*****
TEMPERATURE	397.64	406.66	291.05	359.31	326.46
S. DEW PT.	359.59	378.64	291.74	0.0	0.0
PRESSURE	17.98	17.86	17.67	18.46	18.20

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE - COMPOSITION - MOLES/HR.
ENTHALPY - MMBTU./HR. VOLUME - CU.FT./MIN. (GAS ONLY)
TEMPERATURE - DEG.F. PRESSURE - PSIA.

STREAM NO.	26	27	30	35	36
CH4	0.0	0.0	0.0000	0.0000	0.0000
CO2	0.0	0.0	1710.1897	24.1512	21.0649
O2	0.0	0.0	0.0000	0.0000	0.0000
N2	0.0	0.0	8896.1563	168.9600	135.5030
H2O	0.0	0.0	4000.7864	63.4292	50.5204
H2S	0.0	0.0	4.0386	9.2875	17.9065
SO2	0.0	0.0	84.4457	6.6068	0.8093
S	0.0	0.0	0.0000	0.0052	0.0013
S2	0.0	0.0	0.2023	18.8936	12.5260
S6	0.0	0.0	0.0	0.0000	0.0000
S8	0.0	0.0	0.0	0.0	0.0
COS	0.0	0.0	0.0516	0.3111	0.5529
CS2	0.0	0.0	0.0000	0.0011	0.0040
H2	0.0	0.0	20.8501	11.9072	16.5279
CO	0.0	0.0	9.3141	12.8736	16.7931
S	209.0067	111.0403	0.0	0.0	0.0
TOT. MOLES	209.007	111.040	14726.020	316.426	272.209
TOT. LBS.	6688.2	3553.3	402215.1	9286.2	7629.4
TOT.LB.S(M)	6688.2	3553.3	12.9	1209.4	801.7
TOT.LB.S(E)	6688.2	3553.3	2846.1	1728.0	1418.6
ENTHALPY	0.513	0.241	-564.383	-4.959	-4.322
VOLUME	*****	*****	267883.1	8371.4	6755.6
TEMPERATURE	318.43	287.32	1337.25	2351.11	2177.03
S. DEW PT.	0.0	0.0	251.33	583.79	563.76
PRESSURE	17.98	17.67	17.67	19.00	19.00

EXAMPLE 5.

SPECIFICATIONS

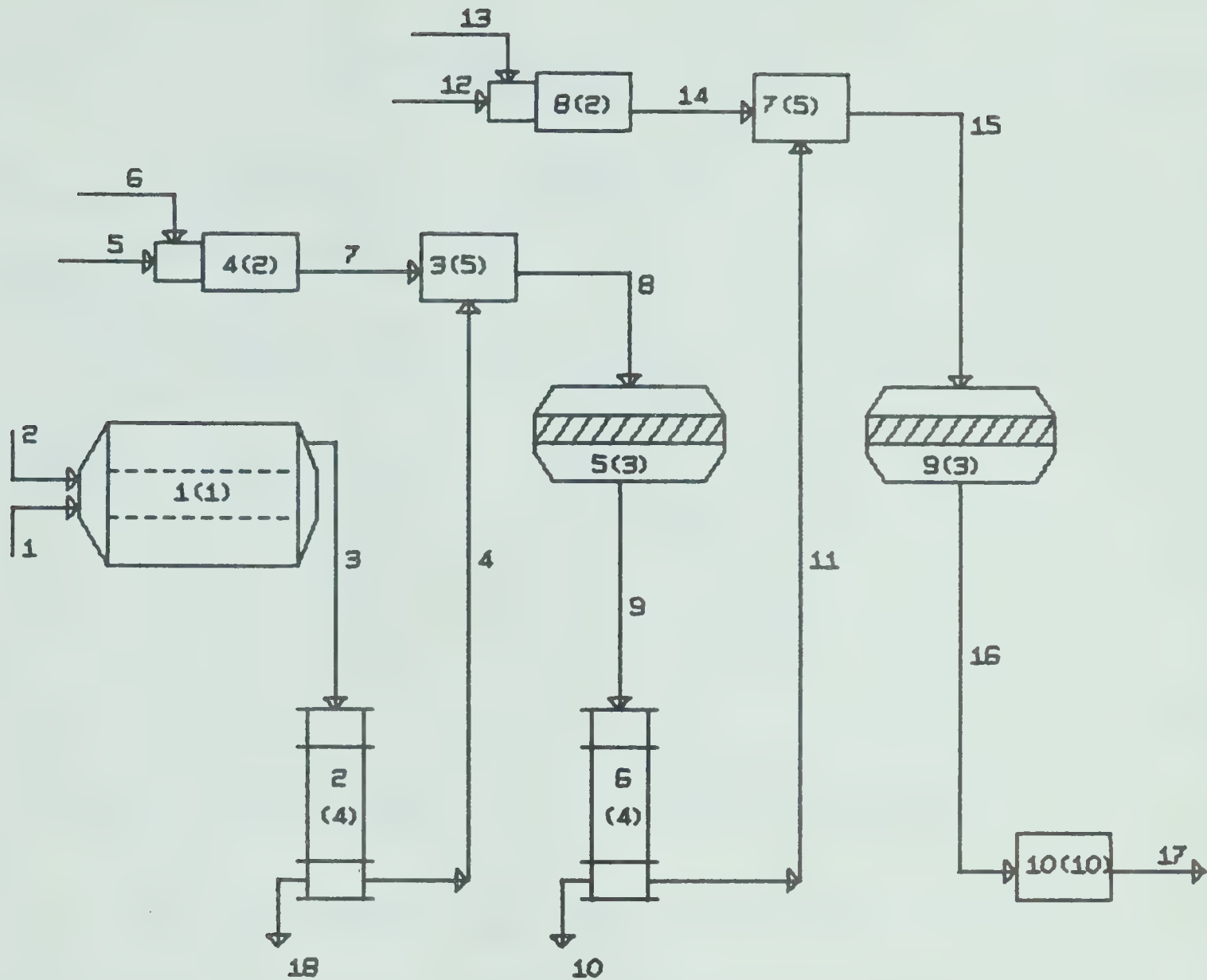
PLANT FEEDS

	BOILER FEED	NO. 1 INLINE BURNER	NO. 2 INLINE BURNER
CH ₄	1.07	0.06	0.03
CO ₂	177.09	10.05	4.29
H ₂ O	10.93	1.0	0.35
H ₂ S	535.48	30.39	12.98
O ₂	250.03	22.85	7.99
N ₂	940.52	85.95	30.05

SPECIFIED TEMPERATURES AND PRESSURES	DEG.F.	PSIA.
BOILER AND INLINE BURNERS ACID GAS FEED	88.	17.2
BOILER AND INLINE BURNER COMBUSTION AIR	88.	18.
BOILER EXIT	700.	
BOILER STEAM		270.
PRIMARY (BOILER) EQUILIBRIUM CUTOFF	2000.	
SECONDARY (MASKING) EQUILIBRIUM CUTOFF	2000.	
NO. 1 CONDENSER EXIT	276.	
NO. 1 CONDENSER STEAM		35.
NO. 2 CONDENSER STEAM		56.
TAIL GAS	274.	15.

MISCELLANEOUS

- 2 PASS BOILER 25. FT. LONG
- MINIMUM FLAME REACTION RESIDENCE TIME 0.6 SEC. (BOILER) AND 0.7 SEC. (INLINE BURNERS)
- NO. 2 CONDENSER - 1122 1.032 IN. DIA. TUBES 16 FT. LONG
- MAX. FOG IN 1ST AND 2ND CONDENSERS 10 AND 5 LB. SULPHUR PER 100 MOLES INERT EXIT GAS RESPECTIVELY



LEGEND

NUMBERS DENOTE STREAM OR EQUIPMENT NUMBERS

NUMBERS IN BRACKETS DENOTE EQUIPMENT TYPES -

- | | |
|------------------------|---------------------|
| 1. WASTE HEAT BOILER | 6. COMBINER/DIVIDER |
| 2. INLINE BURNER | 7. AIR ADDER |
| 3. CATALYTIC CONVERTER | 8. INCINERATOR |
| 4. SULPHUR CONDENSER | 9. EFFLUENT STACK |
| 5. ADIABATIC COMBINER | 10. BLACK BOX |

FIG. E-5 EQUIPMENT MODULE (PROCESS)
FLOWSHEET FOR EXAMPLE 5.

PROGRAM DATA (CARD IMAGE)

```

C          EXAMPLE 5.          (SIMULATION)
*PROGRAM CONTROL PARAMETERS*
      0 0 0 1 0 0 0 0 0 0 0 0 0 0 1
*END*
*FLOWSHEET DATA*
1 0 1**2 0 1**3 1 2**4 2 3**5 0 4**6 0 4**7 4 3**8 3 5**
9 5 6**10 6 0**11 6 7**12 0 8**13 0 8** 14 8 7**15 7 9**
16 9 10**18 2 0**17 10 0**
*END*
*STREAM SPECIFICATIONS*
1      2 177.09 6 535.48 1 1.07 21 88. 22 17.2**
2      3 250.03 4 940.52 5 10.93 21 88. 22 18.**
5      2 10.05 6 30.39 1 .06 21 88. 22 17.2**
6      3 22.85 4 85.95 5 1. 21 88. 22 18.**
12     2 4.29 6 12.98 1 .03 21 88. 22 17.2**
13     3 7.99 4 30.05 5 .35 21 88. 22 20.**
17     21 274. 22 15.**
*END*
*EQUIPMENT PARAMETER SPECIFICATIONS*
1 1, 2 4, 3 5, 4 2, 5 3, 6 4, 7 5, 8 2, 9 3, 10 10, **
1      1 2. 2 25. 10 700. 15 .6 25 2000. 27 270. **
4      3 .7**      8      3 .7**
5      1 1.**      9 1 2.**
6      1 2. 2 16. 3 1.032 4 1122. 5 56. 7 10. 10 10. **
2      1 1. 5 35. 7 18. 8 276. 10 5.**
*END*
C      MOLECULAR AND THERMODYNAMIC DATA SAME AS EXAMPLE 1.

```


SULPHUR PLANT DESIGN AND SIMULATION

PROGRAM CONTROL PARAMETERS

END

FLOWSHEET DATA

END

STREAM SPECIFICATIONS

END

EQUIPMENT PARAMETER SPECIFICATIONS

END

MOLECULAR AND THERMODYNAMIC DATA

END OF ALL DATA

CALCULATION SEQUENCE OPTIMIZATION

INITIAL SEQUENCE IS -

1 2 3 4 5 6 7 8 9 10

THE OPTIMIZED CALCULATION SEQUENCE IS -

1 2 4 3 5 6 8 7 9 10

NO STREAMS NEED BE ASSUMED

PRIMARY REACTION CUT-OFF TEMPERATURE (BOILER) = 2000. DEG.F

SECONDARY REACTION CUT-OFF TEMPERATURE = 2000. DEG.F

(BELOW THIS TEMPERATURE, THE LAST 4 GASEOUS
MOLECULAR SPECIES ARE MASKED FOR THE BOILER
AND THE CONVERTER COMPOSITION CALCULATIONS.)

COMBUSTION REACTION AND WASTE HEAT BOILER.
EQUIPMENT NUMBER 1

CONDENSER 1
EQUIPMENT NUMBER 2

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 700.2 PRESSURE (PSIA) = 16.64
STREAM ENTHALPY (BTU.) = -0.6656891E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	150.29648
O2	-	0.00000	N2	-	940.51978
H2O	-	420.17871	H2S	-	92.72598
SO2	-	58.27095	S	-	0.0
S2	-	3.12584	S6	-	34.39061
S8	-	21.23428	COS	-	1.99660
CS2	-	0.00738	H2	-	35.64478
CO	-	25.85953	S	-	0.0

CONDENSER DESIGN

TUBE LENGTH (FT.) = 23.2
TUBE DIAMETER (IN.) = 1.000
NUMBER OF TUBES = 771

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 4.00
OUTLET GAS TEMPERATURE (DEG.F) = 276.0
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 14.36

EQUIP. HEAT DUTY (BTU/HR.) IS 0.8722928E 07

STEAM TEMP. (DEG.F.) = 259.3
PRESS. (PSIA) = 35.000
LATENT HEAT (BTU/LB) = 941.2
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR.) = 0.9267703E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 99.65, PERCENT RECOVERY = 54.69

SULPHUR FOG - 171.96 MOLES, OR 5502.6 LBS.
SULPHUR LIQUID - 209.19 MOLES, OR 6694.1 LBS.
(STREAM NO. 18 , TEMPERATURE = 264.1 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 5.00

EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 99.65, PERCENT RECOVERY = 98.95

SULPHUR FOG - 2.70 MOLES, OR 86.3 LBS.
SULPHUR LIQUID - 378.45 MOLES, OR 12110.4 LBS.
(STREAM NO. 18 , TEMPERATURE = 269.4 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 4

TEMPERATURE (DEG. F) = 276.0 PRESSURE (PSIA) = 16.42
STREAM ENTHALPY (BTU.) = -0.7611115E 08

MOLE NUMBERS ARE -

CH4	-	0.00000	CO2	-	150.29648
O2	-	0.00000	N2	-	940.51978
H2O	-	420.17871	H2S	-	92.72598
SO2	-	58.27095	S	-	0.0
S2	-	0.00001	S6	-	0.02712
S8	-	0.14467	COS	-	1.99660
CS2	-	0.00738	H2	-	35.64478
CO	-	25.85953	S	-	2.69611

INLINE BURNER.
EQUIPMENT NUMBER 4

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 3

CONVERTER 1
EQUIPMENT NUMBER 5

CONDENSER 2
EQUIPMENT NUMBER 6

EQUIPMENT PROCESS FEED

TEMPERATURE (DEG. F) = 594.1 PRESSURE (PSIA) = 16.32
STREAM ENTHALPY (BTU.) = -0.7816872E 08

MOLE NUMBERS ARE -

CH4	-	0.0	CO2	-	157.64284
O2	-	0.00000	N2	-	1026.46973
H2O	-	519.43750	H2S	-	21.79268
SO2	-	33.31287	S	-	0.0
S2	-	0.38368	S6	-	9.93005
S8	-	8.73762	COS	-	2.04523
CS2	-	0.00747	H2	-	38.82829
CO	-	28.57443	S	-	0.0

CONDENSER SIMULATION

TUBE LENGTH (FT.) = 16.0
TUBE DIAMETER (IN.) = 1.032
NUMBER OF TUBES = 1122

MAXIMUM FLOW RATE (LB/SQ.FT.SEC) = 2.26
OUTLET GAS TEMPERATURE (DEG.F) = 312.9
U (OVERALL) (BTU/HR.SQ.FT.DEG.F) = 8.98

EQUIP. HEAT DUTY (BTU/HR) IS 0.4861012E 07

STEAM TEMP. (DEG.F.) = 288.3
PRESS. (PSIA) = 56.000
LATENT HEAT (BTU/LB) = 919.1
L.H. CORRECTION = 0.0
PRODUCTION (LB/HR) = 0.5288801E 04

CALCULATED SULPHUR OUTLET

PERCENT CONDENSATION = 96.40, PERCENT RECOVERY = 50.36

SULPHUR FOG - 59.96 MOLES, OR 1918.8 LBS.
SULPHUR LIQUID - 65.59 MOLES, OR 2098.9 LBS.
(STREAM NO. 10 , TEMPERATURE = 289.7 DEG.F.)

SPECIFIED MAXIMUM ALLOWABLE FOG FORMATION,
(LBS. S/100 LB. MOLES INERTS) = 10.00

EXISTENCE OF DE-MISTER PADS IS IMPLIED

REVISED SULPHUR OUTLET

PERCENT CONDENSATION = 96.40, PERCENT RECOVERY = 92.01

SULPHUR FOG - 5.71 MOLES, OR 182.8 LBS.
SULPHUR LIQUID - 119.84 MOLES, OR 3834.9 LBS.
(STREAM NO. 10 , TEMPERATURE = 300.3 DEG.F.)

CONDENSER GASEOUS EXIT STREAM
STREAM NUMBER 11

TEMPERATURE (DEG. F) = 312.9 PRESSURE (PSIA) = 16.25
STREAM ENTHALPY (BTU.) = -0.8332501E 08

MOLE NUMBERS ARE -

CH4	-	0.0	CO2	-	157.64284
O2	-	0.00000	N2	-	1026.46973
H2O	-	519.43750	H2S	-	21.79268
SO2	-	33.31287	S	-	0.0
S2	-	0.00010	S6	-	0.11480
S8	-	0.50074	COS	-	2.04523
CS2	-	0.00747	H2	-	38.82829
CO	-	28.57443	S	-	5.71284

INLINE BURNER.
EQUIPMENT NUMBER 8

ADIABATIC STREAM COMBINER
EQUIPMENT NUMBER 7

CONVERTER 2
EQUIPMENT NUMBER 9

TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
395.016	376.685	18.331	16.227
TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
401.087	385.808	15.279	16.205
TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
407.159	393.531	13.628	16.184
TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
413.231	400.249	12.982	16.162
TEMPERATURE IS LESS THAN 25 DEG.F ABOVE DEW POINT.			
419.303	406.215	13.088	16.141

BLACK BOX
EQUIPMENT NUMBER 10

OVERALL PLANT MASS AND ENERGY BALANCE

ATOM AND TOTAL MASS BALANCES

ATOM TYPE	ATOM TOTAL	PERCENT ERROR
S	0.578850E 03	0.00080
O	0.956879E 03	0.00020
C	0.192590E 03	0.00002
H	0.118690E 04	0.00035
N	0.211304E 04	0.0
TOTAL	0.502825E 04	0.00021

ENERGY BALANCE

(ENTHALPY IS RELATIVE AND IN BTU.)

ENTHALPY IN = -0.385697E 08

ENTHALPY OUT = -0.853040E 08

DIFFERENCE = 0.467343E 08

DIFFERENCE SHOULD BE TOTAL PLANT HEAT LOAD

OVERALL PLANT SULPHUR RECOVERY

PERCENT OF TOTAL INLET SULPHUR
OUT AS ELEMENTAL SULPHUR = 94.64

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 1		WASTE HEAT BOILER	
1 =	0.200000E 01 *	2 =	0.250000E 02 *
3 =	0.830000E 02	4 =	0.142000E 03
5 =	0.0	6 =	0.300000E 01 *
7 =	0.250000E 01 *	8 =	0.0
9 =	0.100106E 04	10 =	0.700174E 03 *
11 =	0.0	12 =	0.374150E 00
13 =	0.194979E 00	14 =	0.0
15 =	0.823880E 00 *	16 =	0.474743E 05
17 =	0.240000E 02	18 =	0.720000E 02
19 =	0.0	20 =	0.0
21 =	0.0	22 =	0.0
23 =	0.0	24 =	0.0
25 =	0.200000E 04 *	26 =	0.201848E 04
27 =	0.270000E 03 *	28 =	0.309624E 08

EQUIPMENT NUMBER 2		CONDENSER	
1 =	0.100000E 01 *	2 =	0.232338E 02
3 =	0.100000E 01	4 =	0.771000E 03
5 =	0.350000E 02 *	6 =	0.399957E 01
7 =	0.180000E 02 *	8 =	0.276000E 03 *
9 =	0.0	10 =	0.500000E 01 *
11 =	0.989494E 02	12 =	0.872293E 07

EQUIPMENT NUMBER 4		IN-LINE BURNER	
1 =	0.160000E 02	2 =	0.360000E 02
3 =	0.151795E 01 *	4 =	0.270659E 05
5 =	0.245443E 04		

EQUIPMENT NUMBER 3		ADIABATIC COMBINER	
1 =	0.0	2 =	0.492395E 03
3 =	0.0		

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 5		CONVERTER	
1 =	0.100000E 01 *	2 =	0.335374E 03
3 =	0.300000E 01	4 =	0.100612E 04
5 =	0.964490E-01	6 =	0.100000E 01
7 =	0.185613E 01	8 =	0.500000E 00

EQUIPMENT NUMBER 6		CONDENSER	
1 =	0.200000E 01 *	2 =	0.160000E 02 *
3 =	0.103200E 01 *	4 =	0.112200E 04 *
5 =	0.560000E 02 *	6 =	0.226184E 01
7 =	0.100000E 02 *	8 =	0.312922E 03
9 =	0.0	10 =	0.100000E 02 *
11 =	0.920090E 02	12 =	0.486101E 07

EQUIPMENT NUMBER 8		IN-LINE BURNER	
1 =	0.100000E 02	2 =	0.240000E 02
3 =	0.120326E 01 *	4 =	0.334665E 05
5 =	0.227044E 04		

EQUIPMENT NUMBER 7		ADIABATIC COMBINER	
1 =	0.0	2 =	0.388944E 03
3 =	0.0		

EQUIPMENT NUMBER 9		CONVERTER	
1 =	0.200000E 01 *	2 =	0.305287E 03
3 =	0.300000E 01	4 =	0.915861E 03
5 =	0.107363E 00	6 =	0.100000E 01
7 =	0.205439E 01	8 =	0.500000E 00

EQUIPMENT PARAMETER SUMMARY

PARAMETER NUMBERS AND PARAMETER VALUES
('*' DENOTES PARAMETER VALUE SPECIFICATION)

EQUIPMENT NUMBER 10

BLACK BOX

1 = 0.0

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE -
ENTHALPY - MMBTU./HR.
TEMPERATURE - DEG.F.

COMPOSITION - MOLES/HR.
VOLUME - CU.FT./MIN. (GAS ONLY)
PRESSURE - PSIA.

STREAM NO.	1	2	3	4	5
CH4	1.0700	0.0	0.0000	0.0000	0.0600
CO2	177.0900	0.0	150.2965	150.2965	10.0500
O2	0.0	250.0300	0.0000	0.0000	0.0
N2	0.0	940.5198	940.5198	940.5198	0.0
H2O	0.0	10.9300	420.1787	420.1787	0.0
H2S	535.4797	0.0	92.7260	92.7260	30.3900
SO2	0.0	0.0	58.2710	58.2710	0.0
S	0.0	0.0	0.0	0.0	0.0
S2	0.0	0.0	3.1258	0.0000	0.0
S6	0.0	0.0	34.3906	0.0271	0.0
S8	0.0	0.0	21.2343	0.1447	0.0
COS	0.0	0.0	1.9966	1.9966	0.0
CS2	0.0	0.0	0.0074	0.0074	0.0
H2	0.0	0.0	35.6448	35.6448	0.0
CO	0.0	0.0	25.8595	25.8595	0.0
S	0.0	0.0	0.0	2.6961	0.0
TOT. MOLES	713.640	1201.479	1784.250	1728.367	40.500
TOT. LBS.	26015.4	34532.2	60547.6	48437.0	1476.4
TOT.LB.S(M)	0.0	0.0	12239.0	128.5	0.0
TOT.LB.S(E)	17135.4	0.0	17135.3	5024.8	972.5
ENTHALPY	-34.594	-1.045	-66.569	-76.111	-1.963
VOLUME	4063.8	6537.7	22239.7	13829.9	230.6
TEMPERATURE	88.00	88.00	700.17	276.00	88.00
S. DEW PT.	0.0	0.0	530.72	278.46	0.0
PRESSURE	17.20	18.00	16.64	16.42	17.20

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE -

ENTHALPY - MMBTU./HR.

TEMPERATURE - DEG.F.

COMPOSITION - MOLES/HR.

VOLUME - CU.FT./MIN. (GAS ONLY)

PRESSURE - PSIA.

STREAM NO.	6	7	8	9	10
CH4	0.0	0.0	0.0000	0.0	0.0
CO2	0.0	7.3464	157.6428	157.6428	0.0
O2	22.8500	0.0000	0.0000	0.0000	0.0
N2	85.9500	85.9500	1026.4697	1026.4697	0.0
H2O	1.0000	26.5070	446.6855	519.4375	0.0
H2S	0.0	1.8194	94.5454	21.7927	0.0
SO2	0.0	11.4183	69.6892	33.3129	0.0
S	0.0	0.0046	0.0	0.0	0.0
S2	0.0	8.5495	0.0262	0.3837	0.0
S6	0.0	0.0	1.3840	9.9300	0.0
S8	0.0	0.0	1.5954	8.7376	0.0
COS	0.0	0.0486	2.0452	2.0452	0.0
CS2	0.0	0.0001	0.0075	0.0075	0.0
H2	0.0	3.1835	38.8283	38.8283	0.0
CO	0.0	2.7149	28.5744	28.5744	0.0
S	0.0	0.0	0.0	0.0	119.8404
TOT. MOLES	109.800	147.542	1867.493	1847.161	119.840
TOT. LBS.	3155.8	4632.2	53069.3	53069.2	3834.9
TOT.LB.S(M)	0.0	547.3	675.8	4168.0	3834.9
TOT.LB.S(E)	0.0	972.5	5997.3	5997.3	3834.9
ENTHALPY	-0.096	-2.059	-78.170	-78.169	0.274
VOLUME	597.5	4470.4	19368.7	21329.3	*****
TEMPERATURE	88.00	2454.43	492.39	594.08	300.30
S. DEW PT.	0.0	573.70	372.88	459.79	0.0
PRESSURE	18.00	17.20	16.42	16.32	16.25

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE -

COMPOSITION - MOLES/HR.

ENTHALPY - MMBTU./HR.

VOLUME - CU.FT./MIN. (GAS ONLY)

TEMPERATURE - DEG.F.

PRESSURE - PSIA.

STREAM NO.	11	12	13	14	15
CH4	0.0	0.0300	0.0	0.0000	0.0000
CO2	157.6428	4.2900	0.0	3.3440	160.9868
O2	0.0000	0.0	7.9900	0.0000	0.0000
N2	1026.4697	0.0	30.0500	30.0500	1056.5195
H2O	519.4375	0.0	0.3500	10.9971	530.4346
H2S	21.7927	12.9800	0.0	1.2206	23.0133
SO2	33.3129	0.0	0.0	3.1245	36.4373
S	0.0	0.0	0.0	0.0007	0.0
S2	0.0001	0.0	0.0	4.3019	0.0016
S6	0.1148	0.0	0.0	0.0000	0.6553
S8	0.5007	0.0	0.0	0.0	1.8847
COS	2.0452	0.0	0.0	0.0302	2.0755
CS2	0.0075	0.0	0.0	0.0001	0.0075
H2	38.8233	0.0	0.0	1.1723	40.0006
CO	28.5744	0.0	0.0	0.9457	29.5201
S	5.7128	0.0	0.0	0.0	0.0
TOT. MOLES	1834.438	17.300	38.390	55.187	1881.536
TOT. LBS.	49234.3	630.6	1103.4	1733.9	50968.3
TOT.LB.S(M)	333.0	0.0	0.0	275.3	608.4
TOT.LB.S(E)	2162.4	415.4	0.0	415.4	2577.7
ENTHALPY	-83.325	-0.838	-0.033	-0.872	-84.197
VOLUME	15550.6	98.5	188.0	1566.5	17574.0
TEMPERATURE	312.92	88.00	88.00	2270.44	388.94
S. DEW PT.	314.21	0.0	0.0	597.31	365.37
PRESSURE	16.25	17.20	20.00	17.20	16.25

STREAM COMPOSITION AND PROPERTY SUMMARY.

UNITS ARE -

COMPOSITION - MOLES/HR.

ENTHALPY - MMBTU./HR.

VOLUME - CU.FT./MIN. (GAS ONLY)

TEMPERATURE - DEG.F.

PRESSURE - PSIA.

STREAM NO.	16	17	18
CH4	0.0000	0.0000	0.0
CO2	160.9868	160.9868	0.0
O2	0.0000	0.0000	0.0
N2	1056.5195	1056.5195	0.0
H2O	550.7683	550.7683	0.0
H2S	2.6788	2.6788	0.0
SO2	26.2700	26.2700	0.0
S	0.0	0.0	0.0
S2	0.0050	0.0000	0.0
S6	1.7644	0.4440	0.0
S8	4.8647	5.8563	0.0
COS	2.0755	2.0755	0.0
CS2	0.0075	0.0075	0.0
H2	40.0006	40.0006	0.0
CO	29.5201	29.5201	0.0
S	0.0	0.0	378.4514
TOT. MOLES	1875.460	1875.127	378.451
TOT. LBS.	50968.3	50968.3	12110.4
TOT.LB.S(M)	1584.4	1584.4	12110.4
TOT.LB.S(E)	2577.7	2577.7	12110.4
ENTHALPY	-84.196	-86.340	0.762
VOLUME	18264.7	16402.1	*****
TEMPERATURE	419.30	274.00	269.44
S. DEW PT.	406.21	400.57	0.0
PRESSURE	16.14	15.00	16.42

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